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TERMINAL (ENTER 1, 2, 3, OR ?):2

\*\*\*\*\* Welcome to STN International \*\*\*\*\*

NEWS 1 Web Page for STN Seminar Schedule - N. America  
NEWS 2 AUG 10 Time limit for inactive STN sessions doubles to 40 minutes  
NEWS 3 AUG 18 COMPENDEX indexing changed for the Corporate Source (CS) field  
NEWS 4 AUG 24 ENCOMPLIT/ENCOMPLIT2 reloaded and enhanced  
NEWS 5 AUG 24 CA/CAPLUS enhanced with legal status information for U.S. patents  
NEWS 6 SEP 09 50 Millionth Unique Chemical Substance Recorded in CAS REGISTRY  
NEWS 7 SEP 11 WPIDS, WPINDEX, and WPIX now include Japanese FTERM thesaurus  
NEWS 8 OCT 21 Derwent World Patents Index Coverage of Indian and Taiwanese Content Expanded  
NEWS 9 OCT 21 Derwent World Patents Index enhanced with human translated claims for Chinese Applications and Utility Models  
NEWS 10 NOV 23 Addition of SCAN format to selected STN databases  
NEWS 11 NOV 23 Annual Reload of IFI Databases  
NEWS 12 DEC 01 FRFULL Content and Search Enhancements  
NEWS 13 DEC 01 DGENE, USGENE, and PCTGEN: new percent identity feature for sorting BLAST answer sets  
NEWS 14 DEC 02 Derwent World Patent Index: Japanese FI-TERM thesaurus added  
NEWS 15 DEC 02 PCTGEN enhanced with patent family and legal status display data from INPADOCDB  
NEWS 16 DEC 02 USGENE: Enhanced coverage of bibliographic and sequence information

NEWS EXPRESS MAY 26 09 CURRENT WINDOWS VERSION IS V8.4,  
AND CURRENT DISCOVER FILE IS DATED 06 APRIL 2009.

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\*\*\*\*\* STN Columbus \*\*\*\*\*

FILE 'HOME' ENTERED AT 09:21:19 ON 18 DEC 2009

=> file registry

=>

Uploading C:\Program Files\STNEXP\Queries\10591950-claim 1-v 1.str



chain nodes :  
1 2 3 4 5 6 13 14  
ring nodes :  
7 8 9 10 11 12  
chain bonds :  
1-2 2-3 3-4 4-5 5-6 6-7 10-13 13-14  
ring bonds :  
7-8 7-12 8-9 9-10 10-11 11-12  
exact bonds :  
1-2 2-3 3-4 4-5 5-6 6-7 10-13 13-14  
normalized bonds :  
7-8 7-12 8-9 9-10 10-11 11-12

Match level :  
1:CLASS 2:CLASS 3:CLASS 4:CLASS 5:CLASS 6:CLASS 7:Atom 8:Atom 9:Atom  
10:Atom  
11:Atom 12:Atom 13:CLASS 14:CLASS

L1 STRUCTURE UPLOADED

=> s l1 sss sam  
SAMPLE SEARCH INITIATED 09:22:25 FILE 'REGISTRY'  
SAMPLE SCREEN SEARCH COMPLETED - 43 TO ITERATE

100.0% PROCESSED 43 ITERATIONS 3 ANSWERS  
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*  
BATCH \*\*COMPLETE\*\*  
PROJECTED ITERATIONS: 467 TO 1253  
PROJECTED ANSWERS: 3 TO 163

L2 3 SEA SSS SAM L1

=> d scan

L2 3 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN  
IN 4,9-Dioxo-3,10-disiladodec-6-ene, 6-[[4-[(3E)-3,4-bis[[[(1,1-

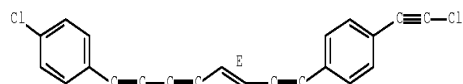
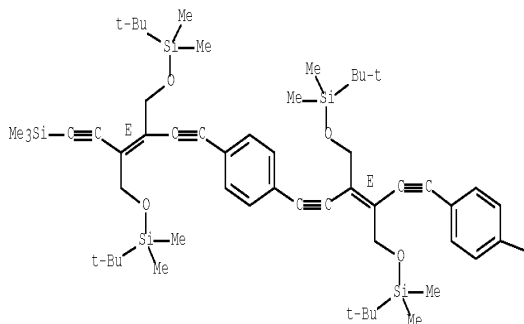


dimethylethyl)dimethylsilyl]oxy)methyl]-6-(4-iodophenyl)-3-hexene-1,5-  
 diynyl]phenyl]ethynyl]-2,2,3,3,10,11,11-octamethyl-7-  
 [(trimethylsilyl)ethynyl]-, (6E)- (9CI)

MF C55 H85 I O4 Si5

Double bond geometry as shown.

PAGE 1-A



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

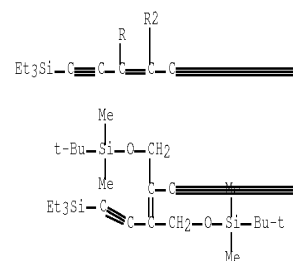
HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L2 3 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN  
 IN Copper(2+), bis[10,13-bis[(3E)-3,4-bis[[[(1,1-dimethylethyl)dimethylsilyl]oxy)methyl]-6-(triethylsilyl)-3-hexene-1,5-diynyl]dipyrido[3,2-a:2',3'-c]phenazine-KN4,KN5]-, (T-4)-, bis[hexafluorophosphate(1-)] (9CI)  
 MF C140 H212 Cu N8 O8 Si12 . 2 F6 P

CM 1

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PAGE 1-B



I

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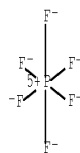
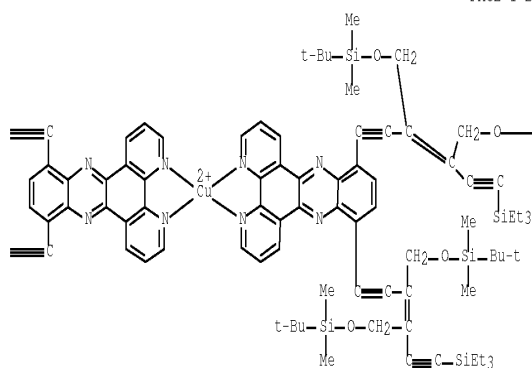
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L2 3 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN  
 IN INDEX NAME NOT YET ASSIGNED  
 MF C22 H10 Cl2

Double bond geometry as shown.



PAGE 1-B



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

ALL ANSWERS HAVE BEEN SCANNED

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FULL SCREEN SEARCH COMPLETED - 765 TO ITERATE

100.0% PROCESSED 765 ITERATIONS 49 ANSWERS  
SEARCH TIME: 00.00.01

L3 49 SEA SSS FUL L1

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C

=> s l3

L4 15 L3

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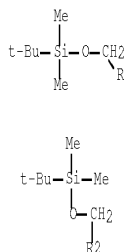
L4 ANSWER 1 OF 15 CAPLUS COPYRIGHT 2009 ACS on STN  
ACCESSION NUMBER: 2009:1167687 CAPLUS [Full-text](#)  
DOCUMENT NUMBER: 151:470282  
TITLE: Synthesis of hybrid masked triyne-phenylene axial rods containing (E)- $\beta$ -chlorovinylsilanes in the  $\pi$ -conjugated framework  
AUTHOR(S): Weller, Michael D.; Kariuki, Benson M.; Cox, Liam R.  
CORPORATE SOURCE: School of Chemistry, The University of Birmingham, Birmingham, B15 2TT, UK  
SOURCE: Journal of Organic Chemistry (2009), 74(20), 7898-7907  
CODEN: JOCEAH; ISSN: 0022-3263  
PUBLISHER: American Chemical Society  
DOCUMENT TYPE: Journal  
LANGUAGE: English

AB Silyl-masked hexayne Me3SiC.tplbond.CC1:C(SiR3)C.tplbond.CC.tplbond.C(SiR3):CC1C.tplbond.CSiMe3 (7, SiR3 = tBuPh2Si) undergoes fluoride-induced  $\beta$ -elimination yielding, after terminal modifications, 1,12-diaryldodecahexaynes; compared to its positional isomer Me3SiC.tplbond.CC(SiR3):CC1C.tplbond.CC.tplbond.CC1:C(SiR3)C.tplbond.CSiMe3 (2, same SiR3), prepared earlier, the compound 7 provides increased flexibility, allowing introduction of aromatic spacer groups, useful in production of carbyne-type mol. wires. A two-directional synthesis of a masked hexayne 7, in which two  $\beta$ -chlorovinylsilanes protect two of the internal alkynes, is reported. The key step involves the Pd-catalyzed oxidative dimerization of alkyne HC.tplbond.CC(SiR3):CC1CH2OTHP (10) to

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provide diyne THPOCH2CCl:C(SiR3)C.tplbond.CC.tplbond.CC(SiR3):CC1CH2OTHP (12), which is elaborated into centrosym. masked hexayne 7 in four steps. Masked hexayne 7 is a constitutional isomer of masked hexayne 2, which has been used as a monomer unit for oligoyne assembly. Although masked hexayne 7 was not as convenient a building block as 2 for application in oligoyne assembly, one of its precursors, namely alkyne 10, could be used successfully in Sonogashira couplings, which allowed the incorporation of aromatic spacers and the formation of hybrid masked triyne-phenylenes

Me3SiC.tplbond.CC(Cl):C(SiR3)C.tplbond.C-1,4-C6H4C.tplbond.CC(SiR3):CC(Cl).CSiMe3 (20) and [Me3SiC.tplbond.CC(Cl):C(SiR3)C.tplbond.C-1,4-C6H4C.tplbond.C]2 (28). Compds. 20 and 28 both contain removable end-groups, which will permit their application as building blocks for the assembly of classes of long-chain,  $\pi$ -conjugated rod-like mols. Rod-like mol.

Me2C(OH)C.tplbond.CC(Cl):C(SiR3)(C.tplbond.CC6H4C.tplbond.C)2C(SiR3):CC(Cl).tpbond.CCMe2(OH) (34, C6H4 = 1,4-phenylene), which possesses a similar conjugated scaffold as 28, was also prepared by using a similar strategy. Treatment of 34 with TBAF effected a 2-fold dechlorosilylation to provide a rigid rod mol. Me2C(OH)(C.tplbond.C)3C6H4(C.tplbond.C)2C6H4(C.tplbond.C)3CMe2(OH) (35) in which two 1,4-phenylene units interrupt an octayne scaffold.

IT 1191093-44-3P 1191093-45-4P 1191093-46-5P

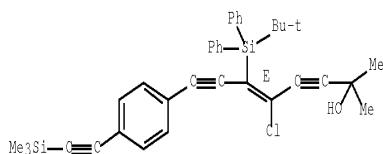
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of  $\pi$ -conjugated p-phenylene-bridged  $\beta$ -chloro silyl-substituted enynes as precursors for arylene-containing polyyne mol. wires)

RN 1191093-44-3 CAPLUS

CN INDEX NAME NOT YET ASSIGNED

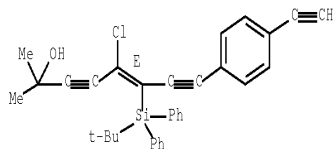
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RN 1191093-45-4 CAPLUS

CN INDEX NAME NOT YET ASSIGNED

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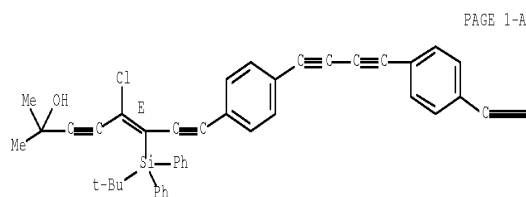


RN 1191093-46-5 CAPLUS

CN 5-Octene-3,7-diyn-2-ol, 8,8'-(1,3-butadiyne-1,4-diyl)-4,1-phenylene)bis[5-chloro-6-[(1,1-dimethylethyl)diphenylsilyl]-2-methyl-, (5E,5'E)- (CA

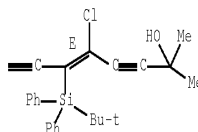
INDEX NAME)

Double bond geometry as shown.



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IT 1191093-33-6P 1191093-41-0P

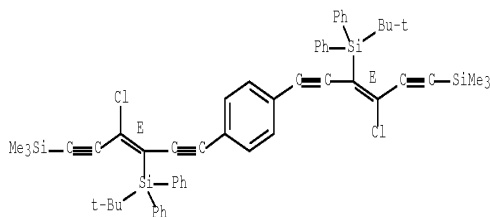
RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation of  $\pi$ -conjugated p-phenylene-bridged  $\beta$ -chloro silyl-substituted enynes as precursors for arylene-containing polyyne mol. wires)

RN 1191093-33-0 CAPLUS

CN Benzene, 1,4-bis[(3E)-4-chloro-3-[(1,1-dimethylethyl)diphenylsilyl]-6-(trimethylsilyl)-3-hexene-1,5-diyn-1-yl]- (CA INDEX NAME)

Double bond geometry as shown.

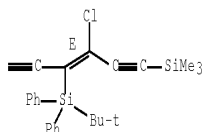
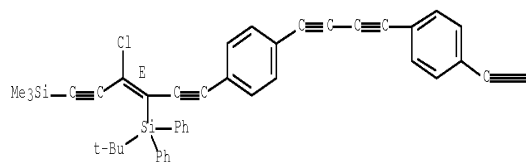


RN 1191093-41-0 CAPLUS

CN Benzene, 1,1'-(1,3-butadiyne-1,4-diyl)bis[4-[(3E)-4-chloro-3-[(1,1-dimethylethyl)diphenylsilyl]-6-(trimethylsilyl)-3-hexene-1,5-diyn-1-yl]- (CA INDEX NAME)

Double bond geometry as shown.





REFERENCE COUNT: 60 THERE ARE 60 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 2 OF 15 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 2005:1004691 CAPLUS [Full-text](#)

DOCUMENT NUMBER: 143:306181

TITLE: Process for preparation of  $\pi$ -conjugated aromatic ring-containing acetylene derivatives as organic electroluminescent devices

INVENTOR(S): Sato, Fumie; Takayama, Yuuki

PATENT ASSIGNEE(S): Nissan Chemical Industries, Ltd., Japan

SOURCE: PCT Int. Appl., 82 pp.

CODEN: PIXXD2

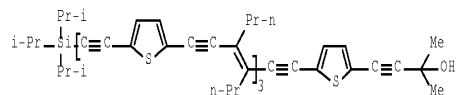
DOCUMENT TYPE: Patent

LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005085176	A1	20050915	WO 2005-JP3950	20050308
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
US 20070176164	A1	20070802	US 2007-591950	20070307
PRIORITY APPLN. INFO.:			JP 2004-65446	A 20040309



AB This invention pertains to a method for producing  $\pi$ -conjugated aromatic ring-containing acetylene derivs. via coupling reaction in the presence of palladium and Cu(I) catalysts. For example, the compound I was prepared in a multi-step synthesis in good yield. The title compds. are useful as electroluminescent devices.

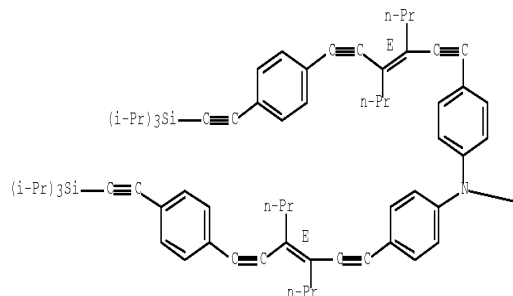
IT 864684-31-1F 864684-32-2F  
RL: IMF (Industrial manufacture); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(intermediate; preparation of  $\pi$ -conjugated aromatic ring-containing acetylene derivs. as organic electroluminescent devices)

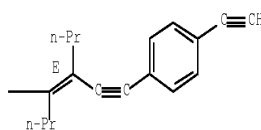
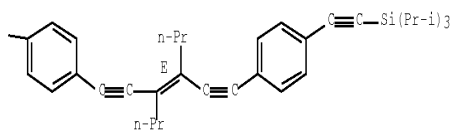
RN 864684-31-1 CAPLUS

CN Benzenamine, N-[4-[(3E)-3,4-dipropyl-6-[4-[2-[tris(1-methylethyl)silyl]ethynyl]phenyl]-4-[(3E)-3-propyl-4-[2-[4-[2-[tris(1-methylethyl)silyl]ethynyl]phenyl]ethynyl]-3-hepten-1-yn-1-yl]-N-[4-[(3E)-3-propyl-4-[2-[4-[2-[tris(1-methylethyl)silyl]ethynyl]phenyl]ethynyl]-3-hepten-1-yn-1-yl]phenyl]- (CA INDEX NAME)

Double bond geometry as shown.







RN 864684-32-2 CAPLUS

CN Benzenamine, N-[4-[(3E)-5-ethyl-4-[2-(4-ethynylphenyl)ethynyl]-3-propyl-3-penten-1-yn-1-yl]phenyl]-4-[(3E)-4-[2-(4-ethynylphenyl)ethynyl]-3-propyl-3-hepten-1-yn-1-yl]-N-[4-[(3E)-4-[2-(4-ethynylphenyl)ethynyl]-3-propyl-3-hepten-1-yn-1-yl]phenyl]- (CA INDEX NAME)

Double bond geometry as shown.

IT 864684-21-9P 864684-22-0P 864684-23-1P

864684-24-2P 864684-25-3P 864684-26-4P

864684-27-5P 864684-28-6P 864684-29-7P

864684-30-8P 864684-33-3P

RL: DEV (Device component use); IMF (Industrial manufacture); SPN (Synthetic preparation); TEM (Technical or engineered material use); PREP (Preparation); USES (Uses)

(preparation of  $\pi$ -conjugated aromatic ring-containing acetylene derivs. as organic

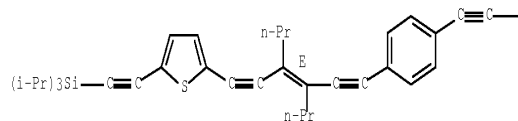
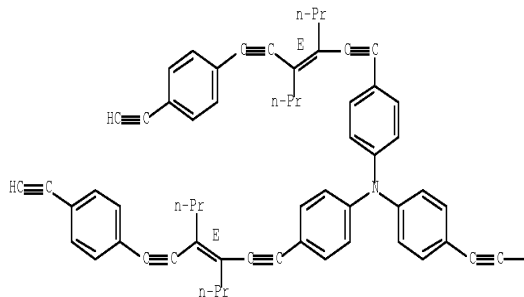
electroluminescent devices)

RN 864684-21-9 CAPLUS

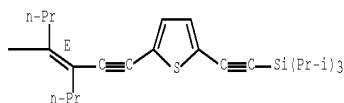
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Double bond geometry as shown.

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RN 864684-22-0 CAPLUS

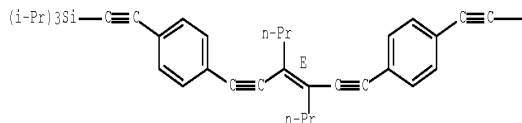
CN Benzene, 1-[(3E)-3,4-dipropyl-6-[4-[2-[tris(1-



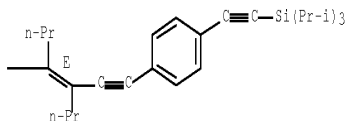
methylethyl)silyl]ethynyl]phenyl]-3-hexene-1,5-diyn-1-yl]-4-[(3E)-3-propyl-4-[2-[4-[2-[tris(1-methylethyl)silyl]ethynyl]phenyl]ethynyl]-3-hepten-1-yn-1-yl]- (CA INDEX NAME)

Double bond geometry as shown.

PAGE 1-A



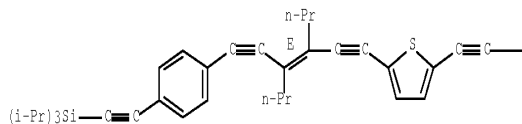
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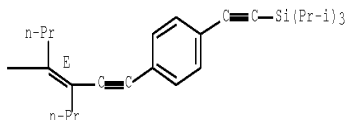
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Double bond geometry as shown.

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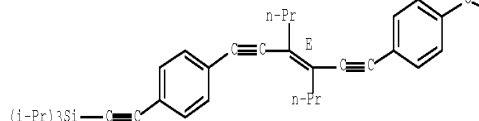
PAGE 1-B



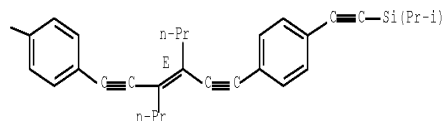
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CN Silane, [oxybis[4,1-phenylene[(3E)-3,4-dipropyl-3-hexene-1,5-diyne-6,1-diyl]-4,1-phenylene-2,1-ethynediyl]]bis[tris(1-methylethyl)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

PAGE 1-A



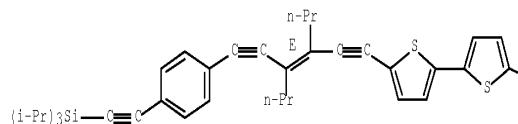
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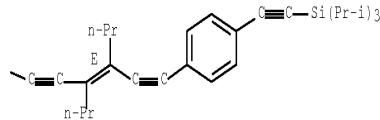
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Double bond geometry as shown.

PAGE 1-A



PAGE 1-B

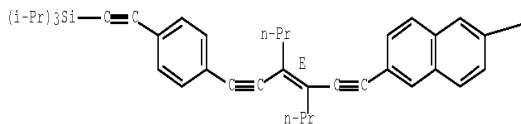




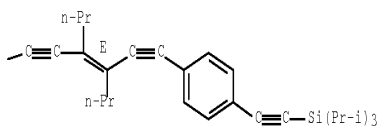
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Double bond geometry as shown.

PAGE 1-A



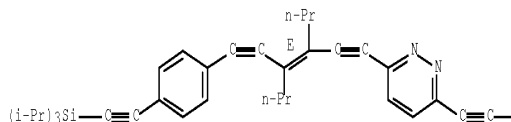
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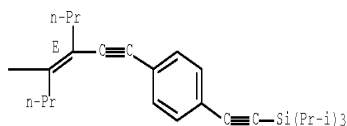
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Double bond geometry as shown.

PAGE 1-A



PAGE 1-B



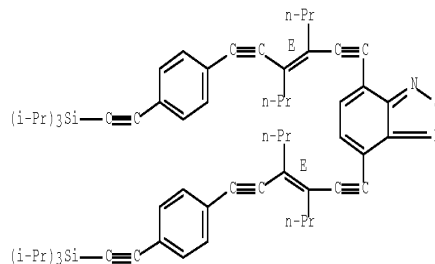
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RN 864684-30-0 CAPLUS  
 CN Benzene, 1-[(3E)-3,4-dipropyl-6-[4-[2-[tris(1-methylethyl)silyl]ethynyl]phenyl]-3-hexene-1,5-diyn-1-yl]-3-[(3E)-5-ethyl-3-propyl-4-[2-[4-[2-[tris(1-methylethyl)silyl]ethynyl]phenyl]ethynyl]-3-penten-1-yn-1-yl]-5-[(3E)-3-propyl-4-[2-[4-[2-[tris(1-methylethyl)silyl]ethynyl]phenyl]ethynyl]-3-hepten-1-yn-1-yl]- (CA INDEX NAME)

Double bond geometry as shown.

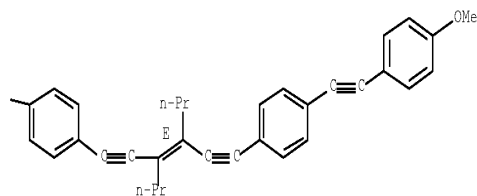
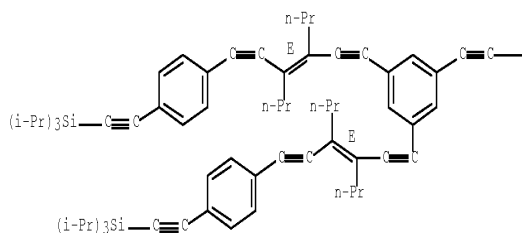
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Double bond geometry as shown.

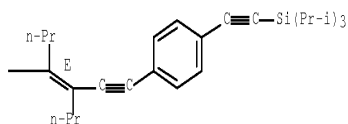




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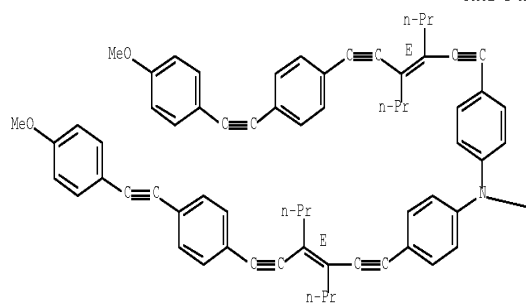
PAGE 1-B



RN 864684-33-3 CAPLUS  
 CN Benzenamine, N-[4-[(3E)-5-ethyl-4-[2-[4-[2-(4-methoxyphenyl)ethynyl]phenyl]ethynyl]-3-propyl-3-penten-1-yn-1-yl]phenyl]-4-[(3E)-4-[2-[4-[2-(4-methoxyphenyl)ethynyl]phenyl]ethynyl]-3-propyl-3-hepten-1-yn-1-yl]-N-[4-[(3E)-4-[2-[4-[2-(4-methoxyphenyl)ethynyl]phenyl]ethynyl]-3-propyl-3-hepten-1-yn-1-yl]phenyl]-(CA INDEX NAME)

Double bond geometry as shown.

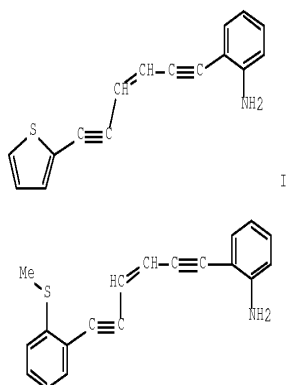
PAGE 1-A



REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 3 OF 15 CAPLUS COPYRIGHT 2009 ACS on STN  
 ACCESSION NUMBER: 2005:354187 CAPLUS [Full-text](#)  
 DOCUMENT NUMBER: 143:333  
 TITLE: Cytotoxicities, cell cycle and caspase evaluations of 1,6-diaryl-3(Z)-hexen-1,5-diynes, 2-(6-aryl-3(Z)-hexen-1,5-diynyl)anilines and their derivatives  
 AUTHOR(S): Lin, Chi-Fong; Lo, Yu-Hsiang; Hsieh, Ming-Chu; Chen, Yi-Hua; Wang, Jeh-Jeng; Wu, Ming-Jung  
 CORPORATE SOURCE: School of Chemistry, Kaohsiung Medical University, Kaohsiung, Taiwan  
 SOURCE: Bioorganic & Medicinal Chemistry (2005), 13(10), 3565-3575  
 CODEN: BMECEP; ISSN: 0968-0896  
 PUBLISHER: Elsevier Ltd.  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 OTHER SOURCE(S): CASREACT 143:333  
 GI

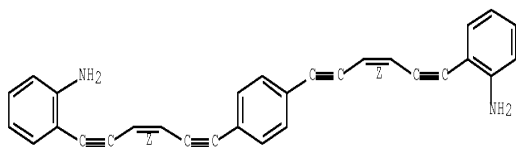




AB A series of compds. showed growth inhibition effects on a full panel of 60 human cancer cell lines, and most of the average IC50 values of the indicated analogs were from <0.01 to 96.6  $\mu$ M, in which a 2-thienyl analog and the thioanisole analog revealed the highest cytotoxic activity with the cancer cell lines at 10-7M concentration range. During the cell cycle anal., a moderate to high apoptotic progress induction was shown by several compared with the control, which 2-(6-(2-thienyl)-3(Z)-hexen-1,5-diynyl)aniline (I) showed the highest apoptotic effect. I and the thioanisole analog displayed a significant G2/M phase arrest in the cell growth cycle compared with other derivs., which the proportions of the G2/M phase cells were accumulated to 71.5% and 82.6%, resp. Moreover, the colorimetric assay of the I and the thioanisole analog also provided advanced evidence to the relationship between the compds. and the caspase-3 enzyme, which was one of the major promoters of apoptotic effect.

IT 852619-13-7P  
 RL: PAC (Pharmacological activity); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)  
 (cytotoxicities, cell cycle and caspase evaluations of  
 1,6-diaryl-3(Z)-hexen-1,5-diyne,  
 2-(6-aryl-3(Z)-hexen-1,5-diynyl)anilines and their derivs.)  
 RN 852619-13-7 CAPLUS  
 CN Benzenamine, 2,2'-[1,4-phenylenedi-(3Z)-3-hexene-1,5-diyne-6,1-diyl]bis-(9CI) (CA INDEX NAME)

Double bond geometry as shown.



OS.CITING REF COUNT: 15 THERE ARE 15 CAPLUS RECORDS THAT CITE THIS RECORD (15 CITINGS)

REFERENCE COUNT: 35 THERE ARE 35 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 4 OF 15 CAPLUS COPYRIGHT 2009 ACS ON STN  
 ACCESSION NUMBER: 2005:17022 CAPLUS Full-text  
 DOCUMENT NUMBER: 142:113747  
 TITLE: Preparation of aryl-substituted acyclic enediyne compounds as antitumor agents  
 INVENTOR(S): Wu, Ming-Jung; Lin, Chi-Fong  
 PATENT ASSIGNEE(S): Kaohsiung Medical University, Taiwan  
 SOURCE: U.S. Pat. Appl. Publ., 41 pp.  
 CODEN: USXXCO  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 2  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 20050004212	A1	20050106	US 2004-847667	20040518
US 7332623	B2	20080219		
CA 2570366	A1	20050317	CA 2004-2570366	20040909
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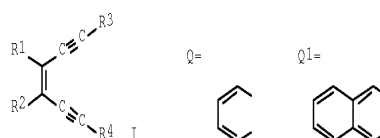
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			US 2003-501266P	P 20030909
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			WO 2004-US29338	W 20040909
			US 2006-488204	A1 20060718

# ASSIGNMENT HISTORY FOR US PATENT AVAILABLE IN LSUS DISPLAY FORMAT

OTHER SOURCE(S): MARPAT 142:113747

GI



AB This invention provides aryl-substituted acyclic enediyne compds. of formula (I) or pharmaceutically acceptable salts or solvates thereof (wherein R1 = R2 = H; or R1 and R2 together form a moiety represented by the formula Q or Q1; R3 = (un)substituted C4-30 alkyl or C3-30 aryl; R4 = (un)substituted C3-30 aryl; with the proviso that R3 is not Bu, pentyl, tetrahydropyranlyoxymethyl, tetrahydropyranlyoxypropyl or Ph when R1 = R2 = H and R4 = o-cyanophenyl; and with the proviso that R3 is not Bu when R1 = R2 = H and R4 = Ph). These compds. found to have inhibitory activities against topoisomerase I or act as a S phase or G2/M phase blocker and were also tested in vitro in anticancer assay. 4-((Z)-3-Dodecen-1,5-diynyl)-1-trifluoromethylbenzene and 2-((Z)-3-dodecen-1,5-diynyl)pyrazine showed IC50 of 4.32 and 5.93 µg/mL against human solid tumor KB cells.

IT

457914-65-7P  
 RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

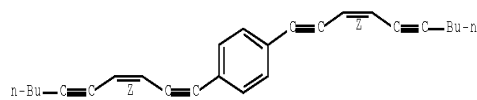
(preparation of aryl-substituted acyclic enediyne compds. as antitumor agents, topoisomerase I inhibitors, or S phase or G2/M phase blockers)

RN 457914-65-7 CAPLUS



CN Benzene, 1,4-di(3Z)-3-decene-1,5-diyn-1-yl- (CA INDEX NAME)

Double bond geometry as shown.



REFERENCE COUNT: 39 THERE ARE 39 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 5 OF 15 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 2005:15944 CAPLUS [Full-text](#)

DOCUMENT NUMBER: 142:113746

TITLE: Preparation of aryl-substituted acyclic enediyne compounds as antitumor agents and pharmaceutical compositions comprising them

INVENTOR(S): Wu, Ming-Jung; Lin, Chi-Fong

PATENT ASSIGNEE(S): Kaohsiung Medical University, Taiwan

SOURCE: U.S. Pat. Appl. Publ., 41 pp.

CODEN: USXXCO

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 2

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 20050004211	A1	20050106	US 2004-847659	20040518
CA 2570366	A1	20050317	CA 2004-2570366	20040909
WO 2005023131	A2	20050317	WO 2004-US29334	20040909
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RU 2336846	C2	20081027	RU 2006-106623	20040909
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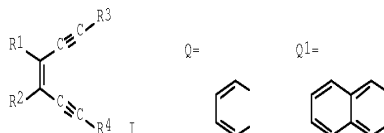


MX 2006002703	A	20060606	MX 2006-2703	20060309
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PRIORITY APPLN. INFO.:

US 2003-483887P	P	20030630
US 2003-501266P	P	20030909
US 2004-832168	A	20040426
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US 2004-847429	A	20040517
US 2004-887644	A	20040709
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JP 2006-524964	A3	20040909
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WO 2004-US29338	W	20040909
US 2006-488204	A1	20060718

OTHER SOURCE(S): MARPAT 142:113746  
GI

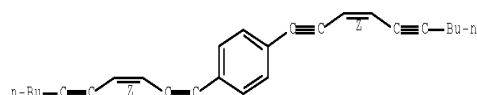


AB A pharmaceutical compns. comprises aryl-substituted acyclic enediyne compds. of formula (I) or pharmaceutically acceptable salts thereof (wherein R1 = R2 = H; or R1 and R2 together form a moiety represented by the formula Q or Q1; R3 = (un)substituted C4-30 alkyl or C3-30 aryl; R4 = (un)substituted C3-30 aryl; with the proviso that R3 is not Bu, pentyl, tetrahydropyranyloxymethyl, tetrahydropyranyloxypropyl or Ph when R1 = R2 = H and R4 = o-cyanophenyl; and with the proviso that R3 is not Bu when R1 = R2 = H and R4 = Ph). The pharmaceutical composition is used to treat a subject afflicted with a tumor/cancer by inhibiting topoisomerase I activities or blocking the S phase or G2/M phase of the tumor/cancer cells. The tumor/cancer cell is selected from leukemia cancer cells, non-small-cell lung cancer cells, col on cancer

cells, CNS cancer cells, melanoma cancer cells, ovarian cancer cells, renal cancer cells, prostate cancer cells and breast cancer cells. These compds. were tested in vitro for inhibitory activities against topoisomerase I, cell cycle at a S phase or G2/M phase blocker, and anticancer growth. For example, 4-((Z)-3-dodecen-1,5-diynyl)-1-trifluoromethylbenzene and 2-((Z)-3-dodecen-1,5-diynyl)pyrazine showed IC50 of 4.32 and 5.93 µg/mL against human solid tumor KB cells.

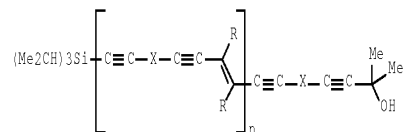
IT 457314-65-7P  
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)  
(preparation of aryl-substituted acyclic enediyne compds. as antitumor agents, topoisomerase I inhibitors, or S phase or G2/M phase blockers)  
RN 457914-65-7 CAPLUS  
CN Benzene, 1,4-di(3Z)-3-decene-1,5-diyn-1-yl- (CA INDEX NAME)

Double bond geometry as shown.



OS.CITING REF COUNT: 3 THERE ARE 3 CAPLUS RECORDS THAT CITE THIS RECORD (4 CITINGS)

L4 ANSWER 6 OF 15 CAPLUS COPYRIGHT 2009 ACS on STN  
ACCESSION NUMBER: 2004:480115 CAPLUS Full-text  
DOCUMENT NUMBER: 141:190674  
TITLE: Synthesis of Conjugated Oligomers Having Aromatic and Eneidyne Units Alternately in the Backbone that Show Intense Fluorescence Emission  
AUTHOR(S): Nakano, Yuuki; Ishizuka, Kenichi; Muraoka, Kenji; Ohtani, Hiroyuki; Takayama, Yuuki; Sato, Fumie  
CORPORATE SOURCE: Department of Biomolecular Engineering, Tokyo Institute of Technology, Midori, Yokohama, Kanagawa, 226-8501, Japan  
SOURCE: Organic Letters (2004), 6(14), 2373-2376  
CODEN: ORLEF7; ISSN: 1523-7060  
PUBLISHER: American Chemical Society  
DOCUMENT TYPE: Journal  
LANGUAGE: English  
OTHER SOURCE(S): CASREACT 141:190674  
GI





AB Synthesis and fluorescence properties of  $\pi$ -conjugated compds. I ( $n = 1 - 3$ ; X = 1,4-phenylene, 2,5-pyridine, 2,5-thiophene; R = n-Pr, n-Bu) having alternately an aromatic or heteroarom. ring and an enediyne unit in the backbone are described.

PAGE 1-B

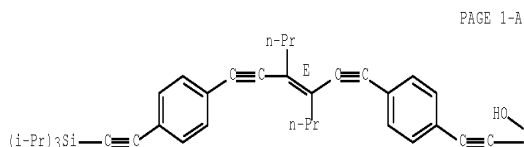
IT 740810-61-1F 740810-62-2P  
 RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and absorption and fluorescence spectra of conjugated oligomers having aromatic (or heteroarom.) and enediyne units alternately in the backbone)

RN 740810-61-1 CAPLUS

CN 3-Butyn-2-ol, 2-methyl-4-[4-[(3E)-3-propyl-4-[2-[4-[2-[tris(1-methylethyl)silyl]ethynyl]phenyl]ethynyl]-3-hepten-1-yn-1-yl]phenyl]- (CA INDEX NAME)

Double bond geometry as shown.



PAGE 1-A

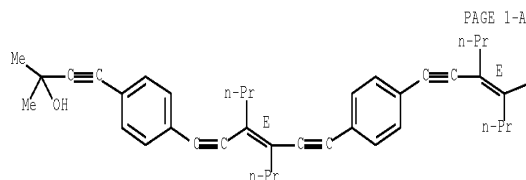
PAGE 1-B



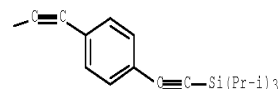
RN 740810-62-2 CAPLUS

CN 3-Butyn-2-ol, 2-methyl-4-[4-[(3E)-3-propyl-4-[4-[(3E)-3-propyl-4-[4-[[tris(1-methylethyl)silyl]ethynyl]phenyl]ethynyl]-3-hepten-1-yn-1-yl]phenyl]ethynyl]-3-hepten-1-yn-1-yl]phenyl]- (CA INDEX NAME)

Double bond geometry as shown.



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IT 740810-63-3P

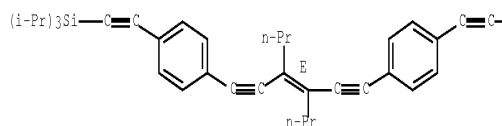
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)  
 (preparation and absorption and fluorescence spectra of conjugated oligomers having aromatic (or heteroarom.) and enediyne units alternately in the backbone)

RN 740810-63-3 CAPLUS

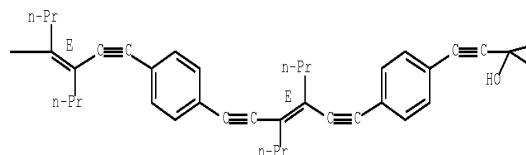
CN 3-Butyn-2-ol, 2-methyl-4-[4-[(3E)-3-propyl-4-[4-[(3E)-3-propyl-4-[4-[[tris(1-methylethyl)silyl]ethynyl]phenyl]ethynyl]-3-hepten-1-yn-1-yl]phenyl]ethynyl]-3-hepten-1-yn-1-yl]phenyl]- (CA INDEX NAME)

Double bond geometry as shown.

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PAGE 1-B



PAGE 1-C



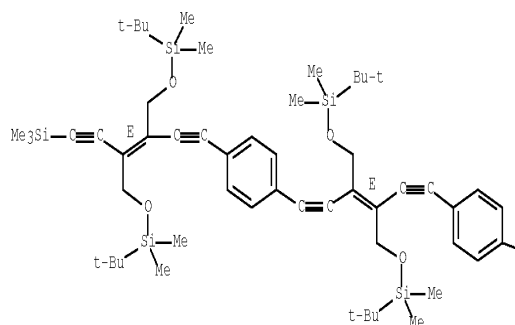


OS.CITING REF COUNT: 20 THERE ARE 20 CAPLUS RECORDS THAT CITE THIS RECORD (20 CITINGS)  
 REFERENCE COUNT: 12 THERE ARE 12 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

Double bond geometry as shown.

PAGE 1-A

L4 ANSWER 7 OF 15 CAPLUS COPYRIGHT 2009 ACS on STN  
 ACCESSION NUMBER: 2004:328526 CAPLUS [Full-text](#)  
 DOCUMENT NUMBER: 141:54000  
 TITLE: Solid-phase synthesis of oligo(triacetylene)s and oligo(phenylenetriacetylene)s employing Sonogashira and Cadiot-Chodkiewicz-type cross-coupling reactions  
 AUTHOR(S): Utesch, Nils F.; Diederich, Francois; Boudon, Corinne; Gisselbrecht, Jean-Paul; Gross, Maurice  
 CORPORATE SOURCE: Laboratorium fuer Organische Chemie, ETH-Hoenggerberg, HCI, Zurich, CH-8093, Switz.  
 SOURCE: Helvetica Chimica Acta (2004), 87(3), 698-718  
 CODEN: HCACAV; ISSN: 0018-019X  
 PUBLISHER: Verlag Helvetica Chimica Acta  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 OTHER SOURCE(S): CASREACT 141:54000



AB The polymer-supported synthesis of poly(triacetylene)-derived monodisperse oligomers is described, using Pd0-catalyzed Sonogashira and Cadiot-Chodkiewicz-type cross-couplings as the key steps in the construction of the acetylenic scaffolds. Merrifield resin functionalized with a 1-(4-iodoaryl)triazene linker was chosen as the polymeric support. The linker selection was made based on the results of several model studies in the liquid phase. For the solid-support synthesis of p-I[C6H4C.tplbond.CC(CH2OSiMe2CM3):C(CH2OSiMe2CM3)C.tplbond.C]nSiMe3 (I, n = 2-4) a set of only three reactions was required: (i) Pd0-catalyzed Sonogashira cross-coupling, (ii) Me3Si-alkyne deprotection by protodesilylation, and (iii) cleavage of the linker with liberation of I. The longest-wavelength absorption maxima of I [n = 1-4] shift bathochromically with increasing oligomeric length, from λmax 337 nm (I, n = 1) to 384 nm (I, n = 4). Based on the electronic absorption data, the effective conjugation length (ECL) of the oligo(phenylene triacetylene)s is estimated to involve at least four monomer units and 40 C-atoms. π-Electron conjugation in these oligomers is less efficient than in Me3Si[C6H4C.tplbond.CC(CH2OSiMe2CM3):C(CH2OSiMe2CM3)C.tplbond.C] nSiMe3 (II) due to poor transmittance of π-electron delocalization by the Ph rings inserted into the oligomeric backbone. Similar conclusions were drawn from the electrochem. properties of the two oligomeric series as determined by cyclic (CV) and rotating-disk voltammetry. In sharp contrast to II, I are strongly fluorescent, with the highest quantum yield ΦF = 0.69 measured for I [n = 3]. Whereas the Sonogashira cross-coupling on solid support proceeded smoothly, optimal conditions for alkyne-alkyne cross-coupling reactions employing Pd0-catalyzed Cadiot-Chodkiewicz conditions still remain to be developed.

PAGE 1-B

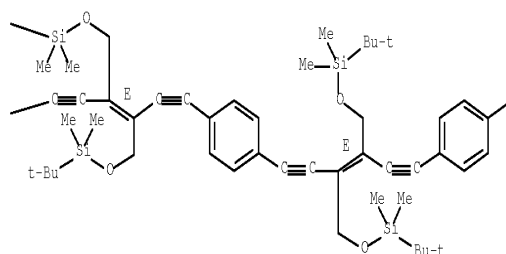
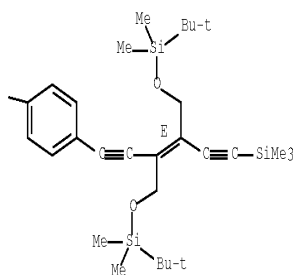
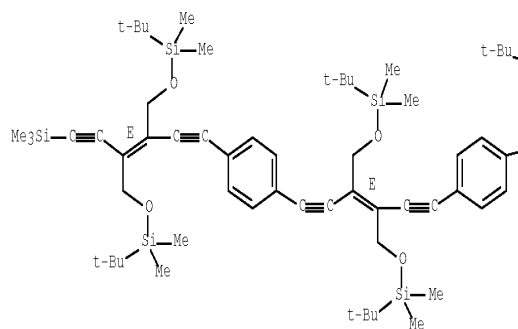
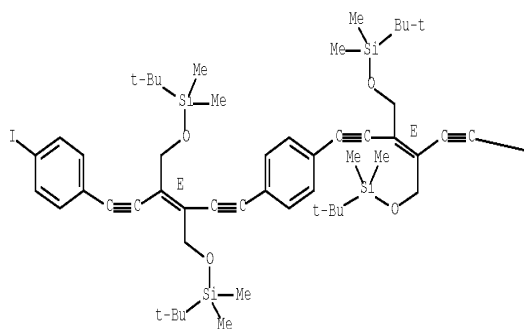
~ I

IT 554459-62-0P 554459-63-1P 554459-64-2P  
 RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)  
 (solid-phase synthesis of oligo(triacetylene)s and oligo(phenylenetriacetylene)s by Sonogashira and Cadiot-Chodkiewicz cross-coupling reactions)  
 RN 554459-62-0 CAPLUS  
 CN 4,9-Dioxa-3,10-disiladodec-6-ene, 6-[[4-[(3E)-3,4-bis[[[(1,1-dimethylethyl)dimethylsilyl]oxy]methyl]-6-(4-iodophenyl)-3-hexene-1,5-diynyl]phenyl]ethynyl]-2,2,3,3,10,10,11,11-octamethyl-7-

RN 554459-63-1 CAPLUS  
 CN 4,9-Dioxa-3,10-disiladodec-6-ene, 6-[[4-[(3E)-6-[4-[(3E)-3,4-bis[[[(1,1-dimethylethyl)dimethylsilyl]oxy]methyl]-6-(4-iodophenyl)-3-hexene-1,5-diynyl]phenyl]-3,4-bis[[[(1,1-dimethylethyl)dimethylsilyl]oxy]methyl]-3-hexene-1,5-diynyl]phenyl]ethynyl]-2,2,3,3,10,10,11,11-octamethyl-7-[(trimethylsilyl)ethynyl]-, (6E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.





RN 554459-64-2 CAPLUS

CN 4,9-Dioxa-3,10-disiladodec-6-ene, 6-[[4-[(3E)-6-[4-[(3E)-3,4-bis[[[(1,1-dimethylethyl)dimethylsilyl]oxy]methyl]-6-(4-iodophenyl)-3-hexene-1,5-diynyl]phenyl]-3,4-bis[[[(1,1-dimethylethyl)dimethylsilyl]oxy]methyl]-3-hexene-1,5-diynyl]phenyl]ethynyl]-7-[[4-[(3E)-3,4-bis[[[(1,1-dimethylethyl)dimethylsilyl]oxy]methyl]-6-(trimethylsilyl)-3-hexene-1,5-diynyl]phenyl]ethynyl]-2,2,3,3,10,10,11,11-octamethyl-, (6E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

IT 704516-23-3P

RL: SPN (Synthetic preparation); PREP (Preparation)

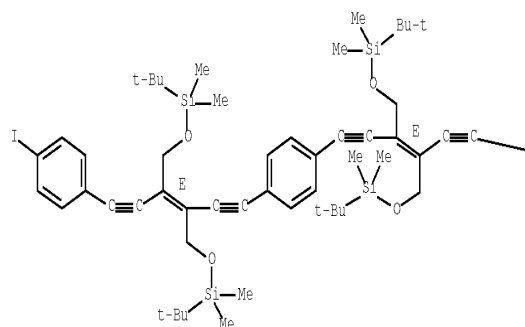
(solid-phase synthesis of oligo(triacetylene)s and oligo(phenylenetriacetylene)s by Sonogashira and Cadiot-Chodkiewicz cross-coupling reactions)

RN 704916-29-0 CAPLUS

CN 4,9-Dioxa-3,10-disiladodec-6-ene, 6,6'-(1,4-phenylenedi-2,1-ethynediyl)bis[7-[(4-iodophenyl)ethynyl]-2,2,3,3,10,10,11,11-octamethyl-, (6E,6'E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.





of a central heterospacer group between two (E)-hex-3-ene-1,5-diyne moieties. A significant increase in the 2nd hyperpolarizability  $\gamma$  is expected if the central spacer fragment is an extended conjugated chromophore. The authors present mols. with enhanced 2nd hyperpolarizability caused by the presence of highly conjugated spacer groups, which increase the overall  $\pi$ -electron delocalization. Some metal complexes obtained from the coordination of these hybrid oligomers to transition-metal centers also were studied and revealed substantial differences in the capacities of the metal centers to act as electronic bridges. Finally, theor. predictions of the relative differences in the 2nd hyperpolarizabilities of the new spacer compds. are in good agreement with the exptl. results.

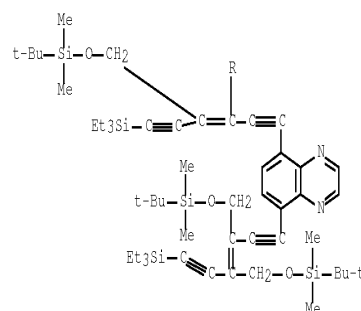
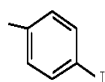
IT 628738-17-0 628738-19-2 628738-20-5

RL: PRP (Properties)

(third-order nonlinear optical properties of in-backbone substituted oligo(triacetylene) chromophores)

RN 628738-17-0 CAPLUS

CN Quinoxaline, 5,8-bis[3,4-bis[[[(1,1-dimethylethyl)dimethylsilyl]oxy]methyl]-6-(triethylsilyl)-3-hexene-1,5-diyne]- (9CI) (CA INDEX NAME)



OS.CITING REF COUNT: 6 THERE ARE 6 CAPLUS RECORDS THAT CITE THIS RECORD (6 CITINGS)  
 REFERENCE COUNT: 93 THERE ARE 93 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 8 OF 15 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 2003:592887 CAPLUS [Full-text](#)

DOCUMENT NUMBER: 140:20929

TITLE: Third-order nonlinear optical properties of in-backbone substituted oligo(triacetylene) chromophores

AUTHOR(S): Concilio, S.; Biaggio, I.; Gunter, P.; Piotto, S. P.; Edelmann, M. J.; Raimundo, J.-M.; Diederich, F.

CORPORATE SOURCE: Swiss Federal Institute of Technology, Institute of Quantum Electronics, Nonlinear Optics Laboratory, ETH-Honggerberg, Zurich, CH-8093, Switz.

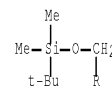
SOURCE: Journal of the Optical Society of America B: Optical Physics (2003), 20(8), 1656-1660  
 CODEN: JOBPDE; ISSN: 0740-3224

PUBLISHER: Optical Society of America

DOCUMENT TYPE: Journal

LANGUAGE: English

AB A new approach to tuning the nonlinear optical properties of hybrid oligo(triacetylene) compds. was studied. The method is based on the insertion

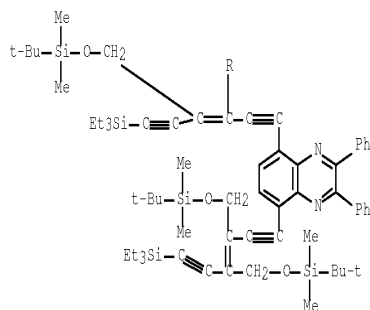


RN 628738-19-2 CAPLUS

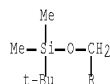
CN Quinoxaline, 5,8-bis[3,4-bis[[[(1,1-dimethylethyl)dimethylsilyl]oxy]methyl]-6-(triethylsilyl)-3-hexene-1,5-diyne-1-yl]-2,3-diphenyl- (CA INDEX NAME)



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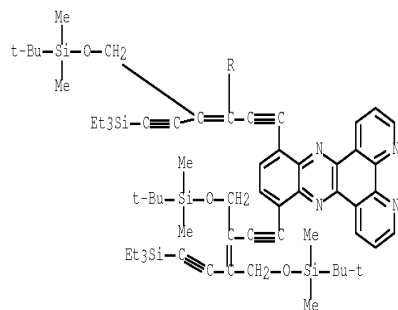


PAGE 2-A

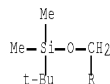


RN 628738-20-5 CAPLUS  
CN Dipyrdo[3,2-a:2',3'-c]phenazine, 10,13-bis[3,4-bis[[[(1,1-dimethylethyl)dimethylsilyl]oxy]methyl]-6-(triethylsilyl)-3-hexene-1,5-diynyl]- (9CI) (CA INDEX NAME)

PAGE 1-A



PAGE 2-A



OS.CITING REF COUNT: 4 THERE ARE 4 CAPLUS RECORDS THAT CITE THIS RECORD (4 CITINGS)  
REFERENCE COUNT: 18 THERE ARE 18 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 9 OF 15 CAPLUS COPYRIGHT 2009 ACS on STN  
ACCESSION NUMBER: 2003:234291 CAPLUS [full-text](#)  
DOCUMENT NUMBER: 139:85055  
TITLE: Acetylenic scaffolding on solid support:  
Poly(triacetylene)-derived oligomers by Sonogashira and Cadiot-Chodkiewicz-type cross-coupling reactions  
AUTHOR(S): Utesch, Nils F.; Diederich, Francois  
CORPORATE SOURCE: Laboratorium fur Organische Chemie, ETH-Honggerberg, HCI, Zurich, CH-8093, Switz.  
SOURCE: Organic & Biomolecular Chemistry (2003), 1(2), 237-239  
CODEN: OBCRAK; ISSN: 1477-0520  
PUBLISHER: Royal Society of Chemistry  
DOCUMENT TYPE: Journal  
LANGUAGE: English  
OTHER SOURCE(S): CASREACT 139:85055

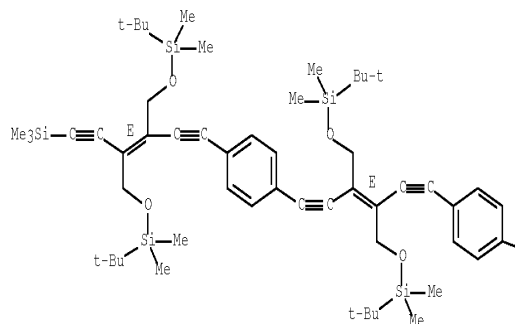
AB Synthesis of poly(triacetylene)-derived oligomers by Pd(0)-catalyzed Sonogashira and Cadiot-Chodkiewicz-type cross-coupling reactions on solid support is reported. Oligo(phenylene triacetylene)s, e.g., I[4-C6H4C.tplbond.CCR:CCR.tplbond.C]nSiMe3 (R = CH2OSiButMe2, n = 1, 2, 3, 4) members of a new class of linearly  $\pi$ -conjugated oligomers with all-C backbones, feature very high fluorescence intensities.

IT 554459-62-0P 554459-63-1P 554459-64-2P  
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)  
(electronic absorption and emission, UV/VIS spectra;  
poly(triacetylene)-derived oligomers are prepared by Sonogashira and Cadiot-Chodkiewicz-type Pd-catalyzed cross-coupling reactions)

RN 554459-62-0 CAPLUS  
CN 4,9-Dioxa-3,10-disiladodec-6-ene, 6-[[4-[(3E)-3,4-bis[[[(1,1-dimethylethyl)dimethylsilyl]oxy]methyl]-6-(4-iodophenyl)-3-hexene-1,5-diynyl]phenyl]ethynyl]-2,2,3,3,10,10,11,11-octamethyl-7-[(trimethylsilyl)ethynyl]-, (6E)- (9CI) (CA INDEX NAME)

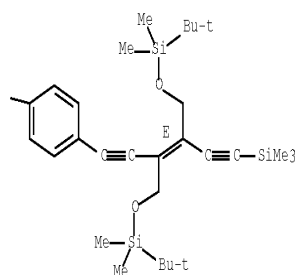
Double bond geometry as shown.

PAGE 1-A





PAGE 1-B



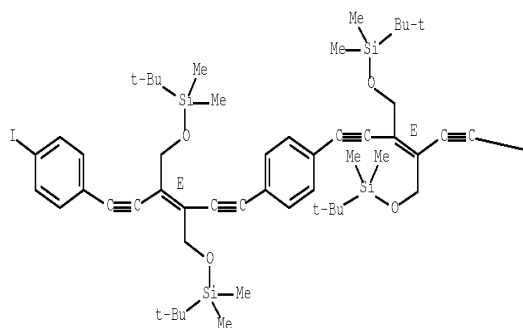
-I

RN 554459-63-1 CAPLUS

CN 4,9-Dioxa-3,10-disiladodec-6-ene, 6-[[4-[(3E)-6-[4-[(3E)-3,4-bis[[[(1,1-dimethylethyl)dimethylsilyl]oxy]methyl]-6-(4-iodophenyl)-3-hexene-1,5-diynyl]phenyl]-3,4-bis[[[(1,1-dimethylethyl)dimethylsilyl]oxy]methyl]-3-hexene-1,5-diynyl]phenyl]ethynyl]-2,2,3,3,10,10,11,11-octamethyl-7-[(trimethylsilyl)ethynyl]-, (6E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

PAGE 1-A

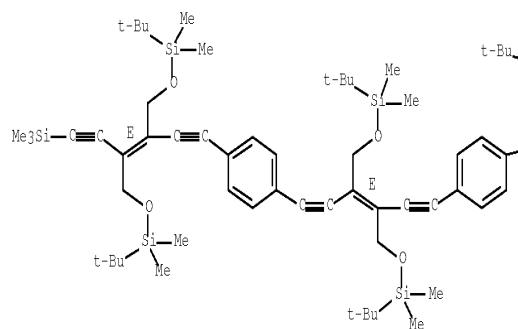


RN 554459-64-2 CAPLUS

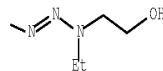
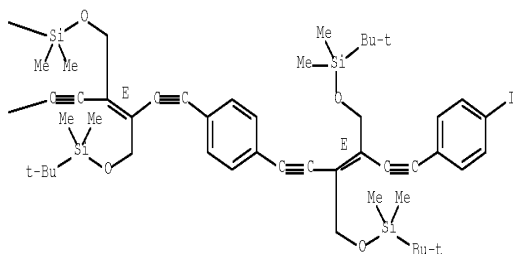
CN 4,9-Dioxa-3,10-disiladodec-6-ene, 6-[[4-[(3E)-6-[4-[(3E)-3,4-bis[[[(1,1-dimethylethyl)dimethylsilyl]oxy]methyl]-6-(4-iodophenyl)-3-hexene-1,5-diynyl]phenyl]-3,4-bis[[[(1,1-dimethylethyl)dimethylsilyl]oxy]methyl]-3-hexene-1,5-diynyl]phenyl]ethynyl]-7-[[4-[(3E)-3,4-bis[[[(1,1-dimethylethyl)dimethylsilyl]oxy]methyl]-6-(trimethylsilyl)-3-hexene-1,5-diynyl]phenyl]ethynyl]-2,2,3,3,10,10,11,11-octamethyl-, (6E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

PAGE 1-A





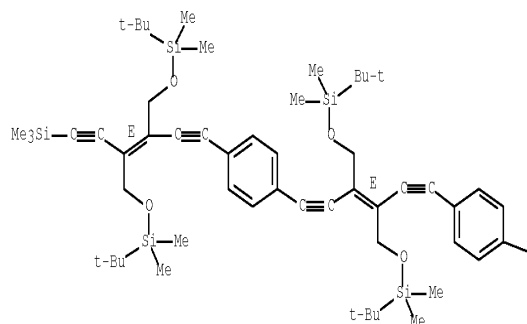


IT 554459-71-1DP, Merrifield resin-supported  
 554459-73-3GP, Merrifield resin-supported 554459-73-3GP  
 , Merrifield resin-supported  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT  
 (Reactant or reagent)  
 (preparation and Sonogashira and Cadiot-Chodkiewicz-type Pd-catalyzed  
 cross-coupling reactions of supported poly(triacetylene)-derived  
 oligomers)

RN 554459-71-1 CAPLUS

CN Ethanol, 2-[3-[4-[(3E)-6-[4-[(3E)-3,4-bis[[[(1,1-dimethylethyl)dimethylsilyl]oxy]methyl]-6-(trimethylsilyl)-3-hexene-1,5-diyn-1-yl]phenyl]-3,4-bis[[[(1,1-dimethylethyl)dimethylsilyl]oxy]methyl]-3-hexene-1,5-diyn-1-yl]phenyl]-1-ethyl-2-triazene-1-yl]- (CA INDEX NAME)

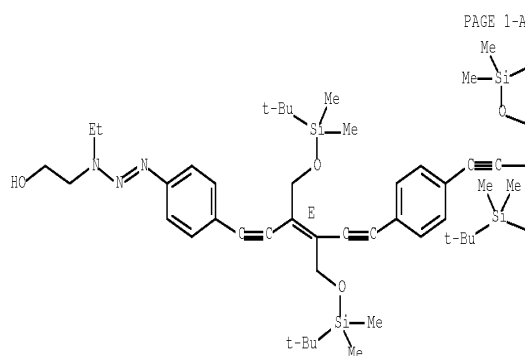
Double bond geometry as described by E or Z.



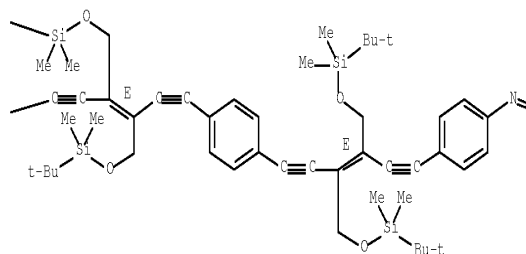
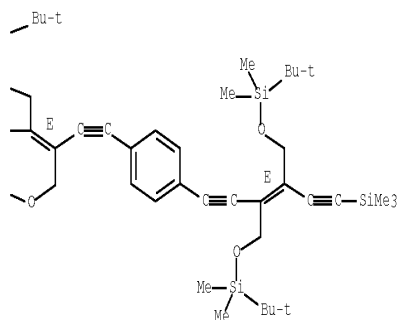
RN 554459-72-2 CAPLUS

CN Ethanol, 2-[3-[4-[(3E)-6-[4-[(3E)-3,4-bis[[[(1,1-dimethylethyl)dimethylsilyl]oxy]methyl]-6-(trimethylsilyl)-3-hexene-1,5-diyn-1-yl]phenyl]-3,4-bis[[[(1,1-dimethylethyl)dimethylsilyl]oxy]methyl]-3-hexene-1,5-diyn-1-yl]phenyl]-1-ethyl-2-triazene-1-yl]- (CA INDEX NAME)

Double bond geometry as described by E or Z.



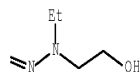




RN 554459-73-3 CAPLUS

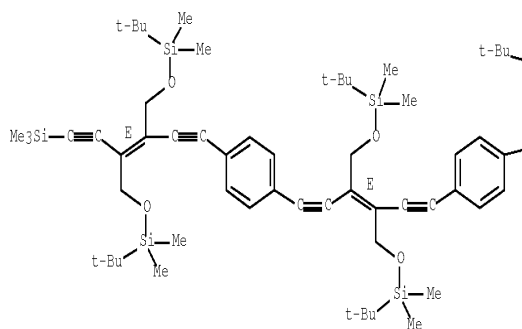
CN Ethanol, 2-[3-[4-[(3E)-6-[4-[(3E)-6-[4-[(3E)-3,4-bis[[[(1,1-dimethylethyl)dimethylsilyl]oxy]methyl]-6-(trimethylsilyl)-3-hexene-1,5-diyn-1-yl]phenyl]-3,4-bis[[[(1,1-dimethylethyl)dimethylsilyl]oxy]methyl]-3-hexene-1,5-diyn-1-yl]phenyl]-3,4-bis[[[(1,1-dimethylethyl)dimethylsilyl]oxy]methyl]-3-hexene-1,5-diyn-1-yl]phenyl]-3,4-bis[[[(1,1-dimethylethyl)dimethylsilyl]oxy]methyl]-3-hexene-1,5-diyn-1-yl]phenyl]-1-ethyl-2-triazen-1-yl]- (CA INDEX NAME)

PAGE 1-C



Double bond geometry as described by E or Z.

PAGE 1-A



OS.CITING REF COUNT: 18 THERE ARE 18 CAPLUS RECORDS THAT CITE THIS RECORD (18 CITINGS)

REFERENCE COUNT: 38 THERE ARE 38 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 10 OF 15 CAPLUS COPYRIGHT 2009 ACS ON STN

ACCESSION NUMBER: 2002:719354 CAPLUS [Full-text](#)

DOCUMENT NUMBER: 138:25161

TITLE: Third-order nonlinear optical properties of in-backbone substituted conjugated polymers

AUTHOR(S): Gubler, U.; Concilio, S.; Bosshard, Ch.; Biaggio, I.; Gunter, P.; Martin, R. E.; Edelmann, M. J.; Wytko, J. A.; Diederich, F.

CORPORATE SOURCE: Institute of Quantum Electronics, ETH-Honggerberg, Zurich, CH-8093, Switz.

SOURCE: Applied Physics Letters (2002), 81(13), 2322-2324 CODEN: APPLAB; ISSN: 0003-6951

PUBLISHER: American Institute of Physics

DOCUMENT TYPE: Journal

LANGUAGE: English

AB An alternative approach for tuning of the third-order nonlinear optical properties of organic mols. is based on insertion a functional group into the path of the  $\pi$ -electron conjugation instead of at chain ends. This scheme enhances the second-order hyperpolarizability for short mols., but in two instances where such mols. were polymerized into longer mols. the overall hyperpolarizability was lower. The study is based on tert-butyl dimethylsilyloxy-vinyl-poly(triacetylene) as the basic linear conjugated polymer, with spacer of anthracene, benzene, naphthalene, thiophene,

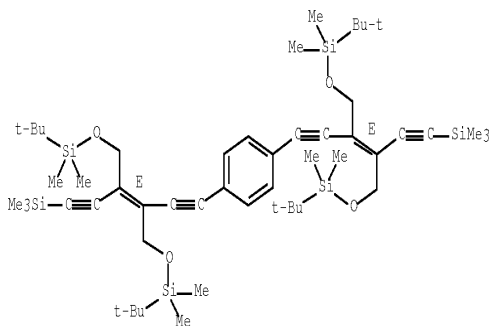


tetramethylbenzene, furan tetrafluorobenzene, pyridine, biphenyl, pyrazine, and bis(triethylphosphine-Pt).

IT 249616-79-3 249616-83-3,  
 9,10-Bis[(E)-3,4-bis[[tert-butyl]dimethylsilyloxy]methyl]-6-(trimethylsilyl)-hex-3-ene-1,5-diynylanthracene 249616-84-0  
 249616-87-3, 1,4-Bis[(E)-3,4-bis[[tert-butyl]dimethylsilyloxy]methyl]-6-(trimethylsilyl)-hex-3-ene-1,5-diynyl]-2,3,5,6-tetramethylbenzene  
 RL: PRP (Properties)  
 (role of in-backbone spacer on third-order nonlinear optical properties of polyacetylene conjugated polymers)

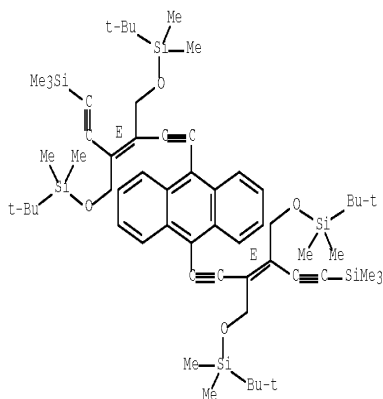
RN 249616-79-3 CAPLUS  
 CN 4,9-Dioxa-3,10-disiladodec-6-ene, 6,6'-(1,4-phenylenedi-2,1-ethynediyl)bis[2,2,3,3,10,10,11,11-octamethyl-7-[(trimethylsilyl)ethynyl]-, (6E,6'E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



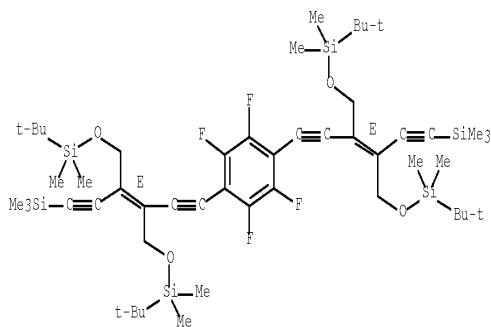
RN 249616-83-9 CAPLUS  
 CN 4,9-Dioxa-3,10-disiladodec-6-ene, 6,6'-(9,10-anthracenediyl)di-2,1-ethynediyl)bis[2,2,3,3,10,10,11,11-octamethyl-7-[(trimethylsilyl)ethynyl]-, (6E,6'E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



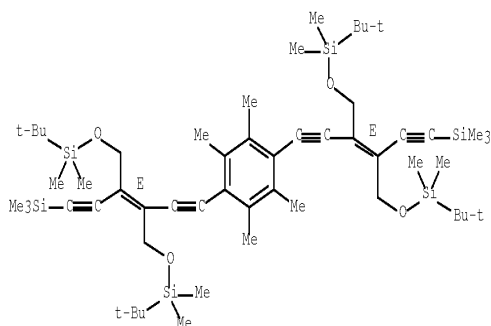
RN 249616-84-0 CAPLUS  
 CN 4,9-Dioxa-3,10-disiladodec-6-ene, 6,6'-[(2,3,5,6-tetrafluoro-1,4-phenylene)di-2,1-ethynediyl]bis[2,2,3,3,10,10,11,11-octamethyl-7-[(trimethylsilyl)ethynyl]-, (6E,6'E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



RN 249616-87-3 CAPLUS  
 CN 4,9-Dioxa-3,10-disiladodec-6-ene, 6,6'-[(2,3,5,6-tetramethyl-1,4-phenylene)di-2,1-ethynediyl]bis[2,2,3,3,10,10,11,11-octamethyl-7-[(trimethylsilyl)ethynyl]-, (6E,6'E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



OS.CITING REF COUNT: 15 THERE ARE 15 CAPLUS RECORDS THAT CITE THIS RECORD (15 CITINGS)  
 REFERENCE COUNT: 11 THERE ARE 11 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 11 OF 15 CAPLUS COPYRIGHT 2009 ACS on STN  
 ACCESSION NUMBER: 2002:700080 CAPLUS [Full-text](#)



DOCUMENT NUMBER: 138:247934  
TITLE: Cytotoxicities and topoisomerase I inhibitory activities of 2-[2-(2-alkynylphenyl)ethynyl]benzonitriles, 1-aryldec-3-ene-1,5-diynes, and related bis(enediynyl)arene compounds  
AUTHOR(S): Lin, Chi-Fong; Lu, Wen-Der; Hsieh, Pei-Chen; Kuo, Yao-Haur; Chiu, Huey-Fen; Wang, Chyi-Jia; Wu, Ming-Jung  
CORPORATE SOURCE: School of Chemistry, Kaohsiung Medical University, Kaohsiung, Taiwan  
SOURCE: Helvetica Chimica Acta (2002), 85(8), 2564-2575  
CODEN: HCACAV; ISSN: 0018-019X  
PUBLISHER: Verlag Helvetica Chimica Acta  
DOCUMENT TYPE: Journal  
LANGUAGE: English  
OTHER SOURCE(S): CASREACT 138:247934

AB The activities of a series of acyclic enediynes, 2-(6-substituted hex-3-ene-1,5-diynyl)benzonitriles (1-5) and their derivs. 7-23 were evaluated against several solid tumor cell lines and topoisomerase I. Comps. 1-5 show selective cytotoxicity with Hepa cells, and 2-[6-phenylhex-3-ene-1,5-diynyl]benzonitrile (5) reveals the most-potent activity. Analogs 8-10 and 13-22 also have the same effect with DLD cells; 1-[(Z)-dec-3-ene-1,5-diynyl]-4-nitrobenzene (21) shows the highest activity among them. Moreover, 1-[(Z)-dec-3-ene-1,5-diynyl]-2- (trifluoromethyl)benzene (20) exhibits the strongest inhibitory activity with the Hela cell line. Derivs. 9, 10, 18, and 23 display inhibitory activities with topoisomerase I at 87  $\mu$ M. The cell-cycle anal. of compound 5, which induces a significant blockage in S phase, indicates that these novel enediynes probably undergo other biol. pathways leading to the cytotoxicity, except the inhibitory activity toward topoisomerase I.

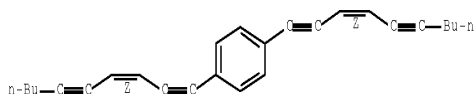
IT 457914-65-7P

RL: PAC (Pharmacological activity); PRP (Properties); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)  
(cytotoxicity and topoisomerase I inhibitory activity of 2-[2-(2-alkynylphenyl)ethynyl]benzonitriles, 1-aryldec-3-ene-1,5-diynes, and related bis(enediynyl)arene compds.)

RN 457914-65-7 CAPLUS

CN Benzene, 1,4-di(3Z)-3-decene-1,5-diyn-1-yl- (CA INDEX NAME)

Double bond geometry as shown.



OS.CITING REF COUNT: 3 THERE ARE 3 CAPLUS RECORDS THAT CITE THIS RECORD (3 CITINGS)

REFERENCE COUNT: 7 THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

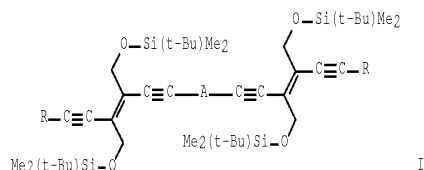
L4 ANSWER 12 OF 15 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 2002:628032 CAPLUS Full-text

DOCUMENT NUMBER: 138:4578

TITLE: Dramatically enhanced fluorescence of heteroaromatic

chromophores upon insertion as spacers into oligo(triacetylene)s  
AUTHOR(S): Edelmann, Michael J.; Raimundo, Jean-Manuel; Utesch, Nils F.; Diederich, Francois  
CORPORATE SOURCE: Lab. Organische Chemie, ETH-Hoenggerberg, HCI, Zurich, CH-8093, Switz.  
SOURCE: Helvetica Chimica Acta (2002), 85(7), 2195-2213  
CODEN: HCACAV; ISSN: 0018-019X  
PUBLISHER: Verlag Helvetica Chimica Acta  
DOCUMENT TYPE: Journal  
LANGUAGE: English  
OTHER SOURCE(S): CASREACT 138:4578  
GI



AB In continuation of a previous study on the modulation of  $\pi$ -electron conjugation of oligo(triacetylene)s by insertion of central hetero-spacer fragments between two (E)-hex-3-ene-1,5-diyne ((E)-1,2-diethynylethene, DEE) moieties, trimeric hybrid oligomers (I; A = spacer, R = SiEt3, SiMe3) were prepared. Spacers used were both electron-deficient (quinoxaline-based heterocycles, pyridazine) and electron-rich (2,2'-bithiophene, 9,9-dioctyl-9H-fluorene)chromophores. With a dipyrrophenazine spacer, transition metal complexes were synthesized as potential precursors for nanoscale scaffolding based on both covalent acetylenic coupling and supramol. assembly. The UV/visible spectra revealed that the majority of spacers provided heterotrimers featuring extended  $\pi$ -electron delocalization. The new hybrid chromophores show a dramatically enhanced fluorescence compared with the DEE dimer and homo-trimer. This increase in emission intensity appears as a general feature of these systems: even if the spacer mol. is nonfluorescent, the corresponding hetero-trimer may show a strong emission. The redox properties of the new hybrid chromophores were determined by cyclic voltammetry (CV) and rotating disk voltammetry (RDV). In each case, the first 1-electron reduction step in the hetero-trimers appeared anodically shifted compared with DEE dimer and homo-trimer. With larger spacer chromophore extending into two dimensions, the anodic shift (by 240-490 mV) seems to originate from inductive effects of the two strongly electron-accepting DEE substituents rather than from extended  $\pi$ -electron conjugation along the oligomeric backbone, as had previously been observed for DEE substituted porphyrins.

IT 477233-33-5P 477234-00-1P 477234-01-2P  
477234-02-3P 477234-04-5P 477234-06-7P  
477234-08-9P

RL: CPS (Chemical process); PEP (Physical, engineering or chemical process); PRP (Properties); SPN (Synthetic preparation); PREP (Preparation); PROC (Process)

(preparation, electrochem. properties and dramatically enhanced fluorescence

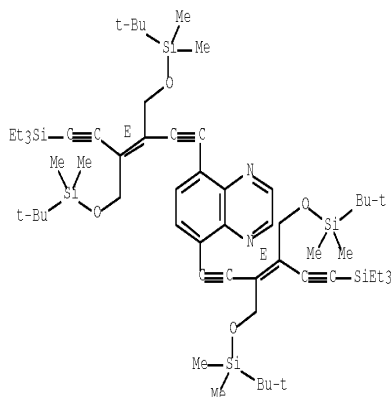


of compds. consisting of heteroarom. chromophores inserted as spacers  
into oligo(triacetylene)s)

RN 477293-99-5 CAPLUS

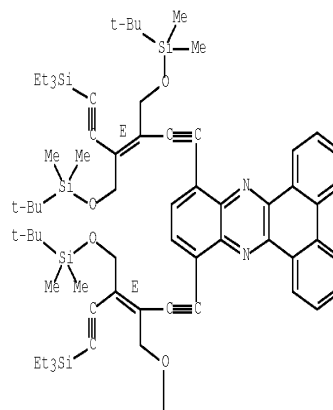
CN Quinoxaline, 5,8-bis[(3E)-3,4-bis[[[(1,1-dimethylethyl)dimethylsilyl]oxy]methyl]-6-(triethylsilyl)-3-hexene-1,5-diynyl]- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



Double bond geometry as shown.

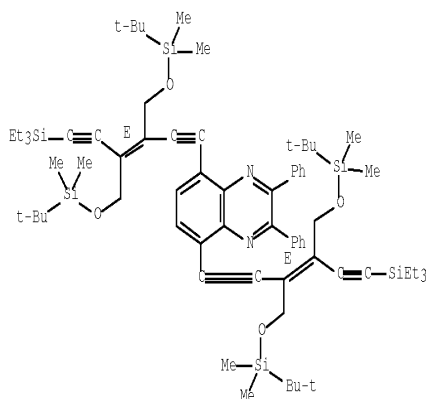
PAGE 1-A



RN 477294-00-1 CAPLUS

CN Quinoxaline, 5,8-bis[(3E)-3,4-bis[[[(1,1-dimethylethyl)dimethylsilyl]oxy]methyl]-6-(triethylsilyl)-3-hexene-1,5-diyn-1-yl]-2,3-diphenyl- (CA INDEX NAME)

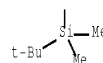
Double bond geometry as shown.



RN 477294-02-3 CAPLUS

CN Dipyrdo[3,2-a:2',3'-c]phenazine, 10,13-bis[(3E)-3,4-bis[[[(1,1-dimethylethyl)dimethylsilyl]oxy]methyl]-6-(triethylsilyl)-3-hexene-1,5-diynyl]- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

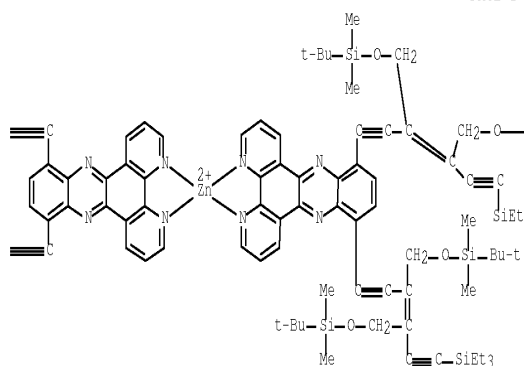
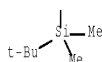
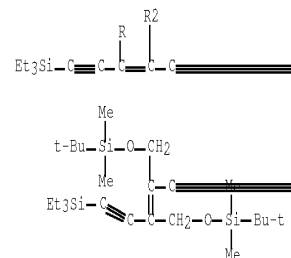
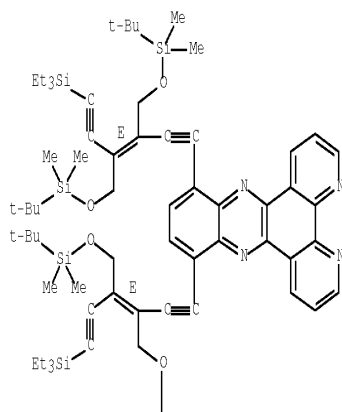


PAGE 2-A

RN 477294-01-2 CAPLUS

CN Dibenzo[a,c]phenazine, 10,13-bis[(3E)-3,4-bis[[[(1,1-dimethylethyl)dimethylsilyl]oxy]methyl]-6-(triethylsilyl)-3-hexene-1,5-diyn-1-yl]- (CA INDEX NAME)





RN 477294-04-5 CAPLUS  
 CN Zinc(2+), bis[10,13-bis[(3E)-3,4-bis[[[(1,1-dimethylethyl)dimethylsilyl]oxy]methyl]-6-(triethylsilyl)-3-hexene-1,5-diynyl]dipyrido[3,2-a:2',3'-c]phenazine- $\kappa\text{N}4,\kappa\text{N}5$ ]-, (T-4)-, salt with trifluoromethanesulfonic acid (1:2) (9CI) (CA INDEX NAME)

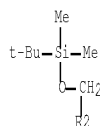
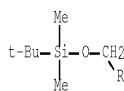
CM 1

CRN 477294-03-4  
 CMF C140 H212 N8 O8 Si12 Zn  
 CCI CCS





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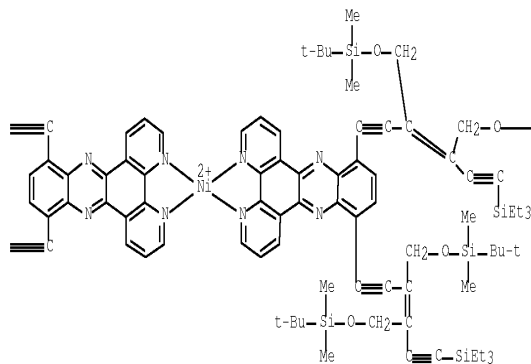
CM 2

CRN 37181-39-8

CMF C F3 O3 S



PAGE 1-B



PAGE 1-C

RN 477294-06-7 CAPLUS

CN Nickel (2+), bis[10,13-bis[(3E)-3,4-bis[[[(1,1-dimethylethyl)dimethylsilyl]oxy]methyl]-6-(triethylsilyl)-3-hexene-1,5-diynyl]dipyrido[3,2-a:2',3'-c]phenazine-KN4,KN5]-, (T-4)-, diperchlorate (9CI) (CA INDEX NAME)

CM 1

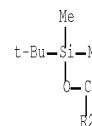
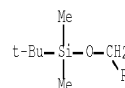
CRN 477294-05-6

CMF C140 H212 N8 Ni O8 Si12

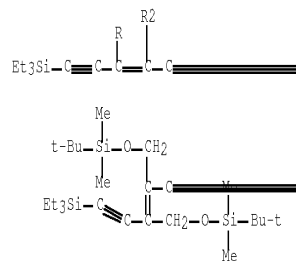
CCI CCS



PAGE 2-A



PAGE 1-A



CM 2

CRN 14797-73-0





RN 477294-08-9 CAPLUS

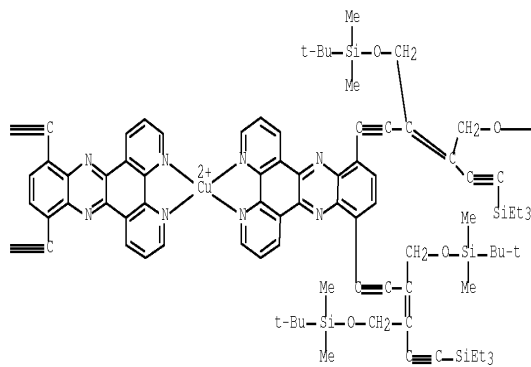
CN Copper(2+), bis[10,13-bis[(3E)-3,4-bis[[[(1,1-dimethylethyl)dimethylsilyl]oxy]methyl]-6-(triethylsilyl)-3-hexene-1,5-diynyl]dipyrido[3,2-a:2',3'-c]phenazine-κN4,κN5]-, (T-4)-, bis[hexafluorophosphate(1-)] (9CI) (CA INDEX NAME)

CM 1

CRN 477294-07-8

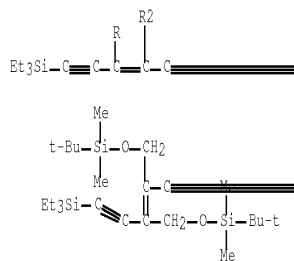
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CCI CCS

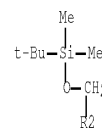
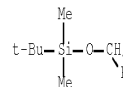


PAGE 1-C

PAGE 1-A



PAGE 2-A



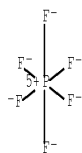
CM 2

CRN 16919-18-9

CMF F6 P

CCI CCS





OS.CITING REF COUNT: 42 THERE ARE 42 CAPLUS RECORDS THAT CITE THIS RECORD (44 CITINGS)

REFERENCE COUNT: 44 THERE ARE 44 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

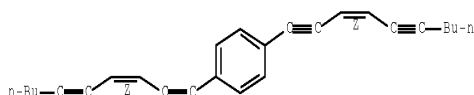
L4 ANSWER 13 OF 15 CAPLUS COPYRIGHT 2009 ACS on STN  
 ACCESSION NUMBER: 2002:539072 CAPLUS [Full-text](#)  
 DOCUMENT NUMBER: 137:232177  
 TITLE: Anionic Cycloaromatization of 1-Aryl-3-hexen-1,5-diynes Initiated by Methoxide Addition: Synthesis of Phenanthridinones, Benzo[c]phenanthridinones, and Biaryls  
 AUTHOR(S): Wu, Ming-Jung; Lin, Chi-Fong; Lu, Wen-Der  
 CORPORATE SOURCE: School of Chemistry, Kaohsiung Medical University, Kaohsiung, Taiwan  
 SOURCE: Journal of Organic Chemistry (2002), 67(17), 5907-5912 CODEN: JOCEAH; ISSN: 0022-3263  
 PUBLISHER: American Chemical Society  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 OTHER SOURCE(S): CASREACT 137:232177

AB Treatment of 2-((Z)-6-substituted-3-hexene-1,5-diynyl)benzonitriles with sodium methoxide in refluxing methanol in the presence of a polar aprotic solvent, such as DMSO, HMPA, THF, or 18-crown-6, gave phenanthridinones in 21-77% yields. In these cases, addition of 10% DMSO into the reaction mixture gave the highest yield. On the other hand, methanolysis of 2-(2-(2-alkynylphenyl)ethynyl)benzonitriles under the same reaction conditions gave benzo[c]phenanthridinones in 31-57% yields. Methanolysis of (Z)-1-aryl-3-hexen-1,5-diynes in the presence of 2 equiv of tetrabutylammonium iodide gave biaryls in 14-64% yields. It is found that the reactions with aryl groups bearing electron-withdrawing groups proceeded at greater rates and gave better yields.

IT 457914-65--??  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
 (anionic cycloaromatization of 1-aryl-3-hexen-1,5-diynes initiated by addition of methanol)

RN 457914-65-7 CAPLUS  
 CN Benzene, 1,4-di(3Z)-3-decene-1,5-diyn-1-yl- (CA INDEX NAME)

Double bond geometry as shown.



OS.CITING REF COUNT: 13 THERE ARE 13 CAPLUS RECORDS THAT CITE THIS RECORD (13 CITINGS)

REFERENCE COUNT: 15 THERE ARE 15 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 14 OF 15 CAPLUS COPYRIGHT 2009 ACS on STN  
 ACCESSION NUMBER: 1999:625317 CAPLUS [Full-text](#)  
 DOCUMENT NUMBER: 131:337377  
 TITLE: Modulation of  $\pi$ -electron conjugation in oligo(triacetylene) chromophores by incorporation of a central spacer  
 AUTHOR(S): Martin, Rainer E.; Wytko, Jennifer A.; Diederich, Francois; Boudon, Corinne; Gisselbrecht, Jean-Paul; Gross, Maurice  
 CORPORATE SOURCE: Laboratorium fur Organische Chemie, ETH-Zentrum, Zurich, CH-8092, Germany  
 SOURCE: Helvetica Chimica Acta (1999), 82(9), 1470-1485 CODEN: HCACAV; ISSN: 0018-019X  
 PUBLISHER: Verlag Helvetica Chimica Acta  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English

AB A series of trimeric hybrid oligomers was prepared by insertion of different hetero-spacers between two (E)-hex-3-ene-1,5-diyne (E = 1,2-diethynylethene, DEE) moieties, and the optical and electrochem. properties of the resulting  $\pi$ -conjugated materials were compared to those of the DEE dimer and trimer, which formally contain a DEE moiety as homo-spacer. The hetero-spacers were: benzenoid (phenylene, naphthalene, biphenylene, anthracene),  $\pi$ -electron-deficient (pyrazine, pyridine) and  $\pi$ -electron-rich (thiophene, furan) aromatic rings, and trans-Pt(PtEt3)2. The hybrid oligomers were synthesized using the method of K. Sonogashira et al. (1978), i.e., cross-coupling between mono-deprotected DEE and the appropriately bis-functionalized spacer. UV/VIS data revealed that the majority of the hetero-spacers were less effective than the homo-spacer DEE in facilitating  $\pi$ -electron delocalization along the linearly conjugated oligomeric backbone. With increasing degree of benzenoid aromaticity in the hetero-spacer, the electronic communication between the terminal DEE moieties in the hybrid oligomers was reduced. As a remarkable exception, a large bathochromic shift of the longest-wavelength absorption maximum, which is indicative of enhanced  $\pi$ -electron delocalization, was obtained upon introducing an anthracene-9,10-diyl moiety as hetero-spacer. Electrochem. studies by cyclic and steady-state voltammetry confirmed the limited extent of  $\pi$ -electron delocalization in the majority of the hybrid oligomers. The fluorescence properties of many of the DEE hybrid materials were dramatically enhanced upon incorporation of the heterospacers. The heterocyclic derivs. containing pyridine, pyrazine, or thiophene spacers, resp., displayed a strong fluorescence emission, demonstrating the value of combining repeat units to modulate oligomeric and polymeric properties. The pyridine derivative provided an interesting example of a mol. system, in which both the electronic absorption and emission characteristics can be reversibly switched as a function of pH.

IT 249616-79-3P, 4-Bis[(E)-3,4-bis[[[(tert-butyl)dimethylsilyloxy]methyl]-6-(trimethylsilyl)-hex-3-ene-1,5-diynyl]benzene 249616-83-3P, 9,10-Bis[(E)-3,4-bis[[[(tert-butyl)dimethylsilyloxy]methyl]-6-(trimethylsilyl)-hex-3-ene-1,5-diynyl]anthracene 249616-84-0P 249616-87-3P, 1,4-Bis[(E)-3,4-bis[[[(tert-butyl)dimethylsilyloxy]methyl]-6-(trimethylsilyl)-hex-3-ene-1,5-diynyl]-2,3,5,6-tetramethylbenzene  
 RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)

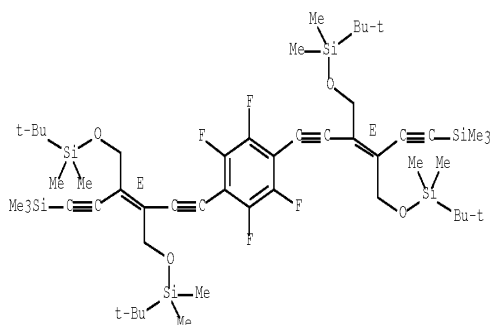
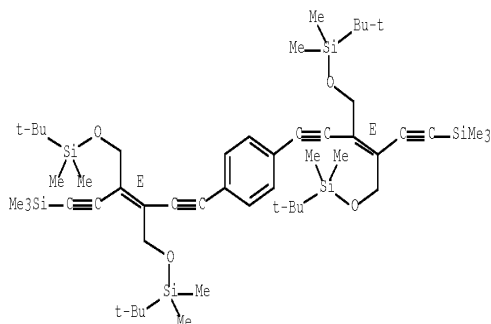


(preparation and modulation of  $\pi$ -electron conjugation in oligoacetylene chromophores by central spacer with variable electron d.)

RN 249616-79-3 CAPLUS

CN 4,9-Dioxa-3,10-disiladodec-6-ene, 6,6'-(1,4-phenylenedi-2,1-ethynediyl)bis[2,2,3,3,10,10,11,11-octamethyl-7-[(trimethylsilyl)ethynyl]-, (6E,6'E)- (9CI) (CA INDEX NAME)

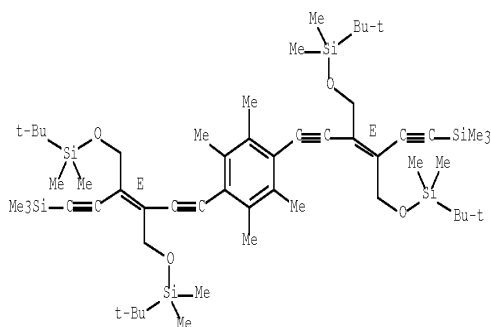
Double bond geometry as shown.



RN 249616-87-3 CAPLUS

CN 4,9-Dioxa-3,10-disiladodec-6-ene, 6,6'-[(2,3,5,6-tetramethyl-1,4-phenylene)di-2,1-ethynediyl]bis[2,2,3,3,10,10,11,11-octamethyl-7-[(trimethylsilyl)ethynyl]-, (6E,6'E)- (9CI) (CA INDEX NAME)

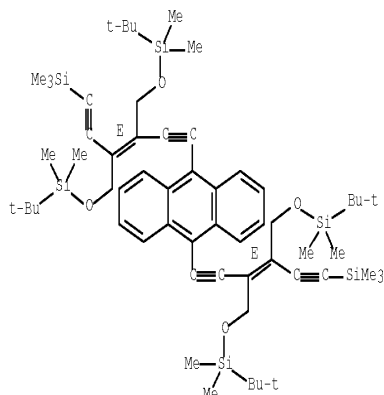
Double bond geometry as shown.



RN 249616-83-9 CAPLUS

CN 4,9-Dioxa-3,10-disiladodec-6-ene, 6,6'-(9,10-anthracenediyl)di-2,1-ethynediyl)bis[2,2,3,3,10,10,11,11-octamethyl-7-[(trimethylsilyl)ethynyl]-, (6E,6'E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



OS.CITING REF COUNT: 29 THERE ARE 29 CAPLUS RECORDS THAT CITE THIS RECORD (29 CITINGS)  
REFERENCE COUNT: 69 THERE ARE 69 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 15 OF 15 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1968:78330 CAPLUS [Full-text](#)

DOCUMENT NUMBER: 68:78330

ORIGINAL REFERENCE NO.: 68:15123a,15126a

TITLE: Interaction of diiodoethylene with copper acetylides

AUTHOR(S): Ukhin, L. Yu.; Sladkov, A. M.; Gorshkov, V. I.

CORPORATE SOURCE: Inst. Elementoorg. Soedin, Moscow, USSR

SOURCE: Zhurnal Organicheskoi Khimii (1968), 4(1), 25-7

CODEN: ZORKAE; ISSN: 0514-7492

DOCUMENT TYPE: Journal

LANGUAGE: Russian

RN 249616-84-0 CAPLUS

CN 4,9-Dioxa-3,10-disiladodec-6-ene, 6,6'-[(2,3,5,6-tetrafluoro-1,4-phenylene)di-2,1-ethynediyl]bis[2,2,3,3,10,10,11,11-octamethyl-7-[(trimethylsilyl)ethynyl]-, (6E,6'E)- (9CI) (CA INDEX NAME)

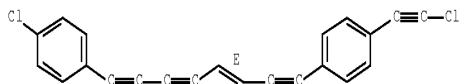
Double bond geometry as shown.



AB Reaction of trans-diiodoethylene (I) with Cu acetylides gave the condensation products of general formula RC.tplbond.CCH:CHI (IIa) or RC.tplbond.CCH:CHC.tplbond.CR (IIb). The structure of products was confirmed by ir and mass spectroscopy; trans configuration of the double bond was preserved. For example, a mixture of 3.29 g. (PhC.tplbond.C)2Cu, 2.78 g. I, and 100 ml. HCONMe2 was stirred 4 hrs. at 90° and then refluxed 2 hrs. Cooling, filtration, and addition of H2O to the filtrate precipitated 56% IIb (R = Ph) m. 111-12° (heptane). Similarly, IIb (R = Bu) b4 117°, n24D 1.5173 was prepared Boiling 23.4 g. (BuC.tplbond.C)2Cu with 44.8 g. I in 125 ml. pyridine for 10 min. gave 40% IIa (R = Bu) b5 84-5°, n20D 1.5519. Similarly IIa (R = Ph) b2.5 112-14°, n23D 1.6880 was prepared However boiling (p-IC6H4C.tplbond.C)2Cu, with I in pyridine gave IIa (R = p-IC6H4) m. 125-30° and IIb (R = p-IC6H4) m. 245-7° (C6H6-heptane), separated by crystallization Also (p-ClC6H4C.tplbond.C)2Cu and I gave IIa (R = p-ClC6H4C.tplbond.C) m. 80-5° and IIb (R = p-ClC6H4C.tplbond.C) m. 179-85° (heptane). To further confirm the structures of IIa and IIb they were converted to boranes by refluxing with an excess of decaborane in PhMe solution The following were characterized (compound, % yield, and m.p. given): 1,2-bis(1-butylborenyl)ethylene, 62, 153-5° (PhMe); 1-(β-iodovinyl)-2-phenylbarene, -, 227-35° (hexane); 1-(β-iodovinyl)-2-butylbarene, -, 72-4°.

IT 1082669-94-0P  
 RL: SPN (Synthetic preparation); PRP (Properties); PREP (Preparation)  
 (Interaction of diiodoethylene with copper acetylides)  
 RN 1082669-94-0 CAPLUS  
 CN INDEX NAME NOT YET ASSIGNED

Double bond geometry as shown.



=>  
 => file registry

=>  
 Uploading C:\Program Files\STNEXP\Queries\10591950-claim 1-v 2.str



chain nodes :  
 1 2 3 4 5 6 7 8 9

chain bonds :  
 1-2 2-3 3-4 4-5 5-6 6-7 7-8 8-9  
 exact/norm bonds :  
 6-7 7-8  
 exact bonds :  
 1-2 2-3 3-4 4-5 5-6 8-9

G1:Cb,Cy,Hy

Match level :  
 1:CLASS 2:CLASS 3:CLASS 4:CLASS 5:CLASS 6:CLASS 7:Atom 8:CLASS 9:CLASS

L5 STRUCTURE UPLOADED

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 SAMPLE SCREEN SEARCH COMPLETED - 408 TO ITERATE

100.0% PROCESSED 408 ITERATIONS 4 ANSWERS  
 SEARCH TIME: 00.00.01

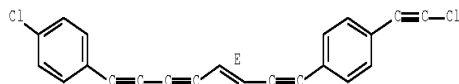
FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*  
 BATCH \*\*COMPLETE\*\*  
 PROJECTED ITERATIONS: 6949 TO 9371  
 PROJECTED ANSWERS: 4 TO 200

L6 4 SEA SSS SAM L5

=> d scan

L6 4 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN  
 IN INDEX NAME NOT YET ASSIGNED  
 MF C22 H10 Cl2

Double bond geometry as shown.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

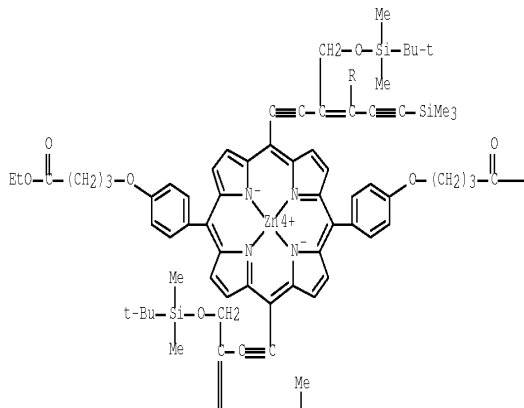
HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L6 4 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN  
 IN Zinc(2+), [[diethyl 4,4'-[[[10,20-bis[(3E)-3,4-bis[[[(1,1-dimethylethyl)dimethylsilyl]oxy]methyl]-6-(trimethylsilyl)-3-hexene-1,4-dienyl]-21H,23H-porphine-5,15-diyl-κN21,κN22,κN23,κN24]bis(4,1-



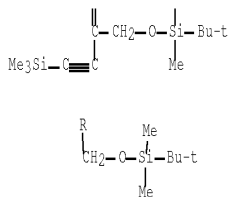
phenyleneoxy]]bis[butanoato]](2-)]-, (SP-4-1)- (9CI)  
 MF C90 H124 N4 O10 Si6 Zn  
 CI CCS

PAGE 1-A



PAGE 1-B

-OEt

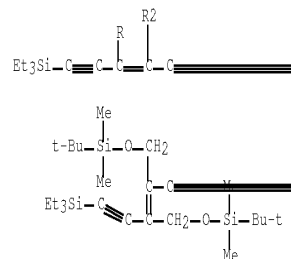


PAGE 2-A

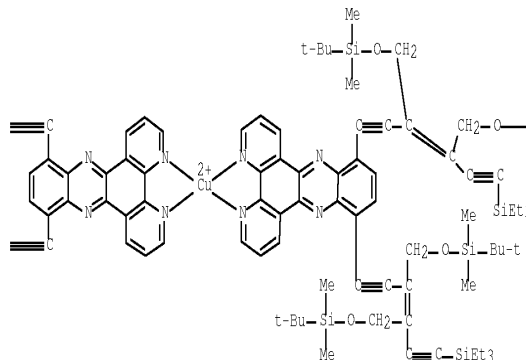
L6 4 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN  
 IN Copper(2+), bis[10,13-bis[(3E)-3,4-bis[[[(1,1-dimethylethyl)dimethylsilyl]oxy]methyl]-6-(triethylsilyl)-3-hexene-1,5-diynyl]dipyrido[3,2-a:2',3'-c]phenazine-KN4,KN5]-, (T-4)-, bis[hexafluorophosphate(1-)] (9CI)  
 MF C140 H212 Cu N8 O8 Si12 . 2 F6 P

CM 1

PAGE 1-A

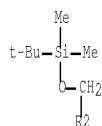
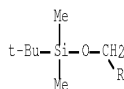
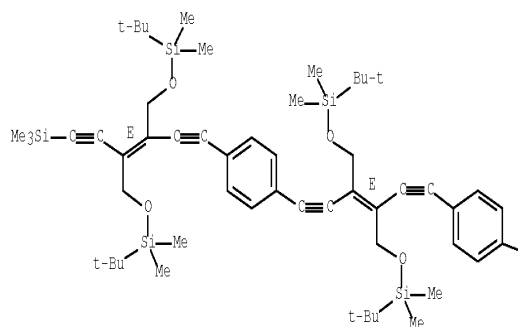


PAGE 1-B

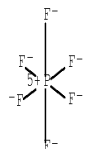


HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1





CM 2



-I

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

ALL ANSWERS HAVE BEEN SCANNED

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

=> s 15 sss full  
 FULL SEARCH INITIATED 09:41:46 FILE 'REGISTRY'  
 FULL SCREEN SEARCH COMPLETED - 7813 TO ITERATE

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

100.0% PROCESSED 7813 ITERATIONS 123 ANSWERS  
 SEARCH TIME: 00.00.01

L6 4 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN  
 IN 4,9-Dioxa-3,10-disiladodec-6-ene, 6-[[4-[(3E)-3,4-bis[[[(1,1-dimethylethyl)dimethylsilyl]oxy]methyl]-6-(4-iodophenyl)-3-hexene-1,5-diynyl]phenyl]ethynyl]-2,2,3,3,10,10,11,11-octamethyl-7-[(trimethylsilyl)ethynyl]-, (6E)- (9CI)  
 MF C55 H85 I O4 Si5

L7 123 SEA SSS FUL L5

=&gt; file caplus

Double bond geometry as shown.

=> s 17  
 L8 39 L7



=> d ibib abs hitstr 1-

YOU HAVE REQUESTED DATA FROM 39 ANSWERS - CONTINUE? Y/(N):y

L8 ANSWER 1 OF 39 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 2009:1167687 CAPLUS Full-text

DOCUMENT NUMBER: 151:470282

TITLE: Synthesis of hybrid masked triyne-phenylene axial rods containing (E)- $\beta$ -chlorovinylsilanes in the

$\pi$ -conjugated framework

AUTHOR(S): Weller, Michael D.; Kariuki, Benson M.; Cox, Liam R.

CORPORATE SOURCE: School of Chemistry, The University of Birmingham, Birmingham, B15 2TT, UK

SOURCE: Journal of Organic Chemistry (2009), 74(20), 7898-7907  
CODEN: JOCEAH; ISSN: 0022-3263

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Silyl-masked hexayne Me3SiC.tplbond.CC(Cl)C(SiR3)C.tplbond.CC.tplbond.C(SiR3):CC(Cl)C.tplbond.CSiMe3 (7, SiR3 = tBuPh2Si) undergoes fluoride-induced  $\beta$ -elimination yielding, after terminal modifications, 1,12-diaryldodecahexaynes; compared to its positional isomer

Me3SiC.tplbond.CC(SiR3):CC(Cl)C.tplbond.CC.tplbond.CC(Cl)C(SiR3)C.tplbond.CSiMe3 (2, same SiR3), prepared earlier, the compound 7 provides increased flexibility, allowing introduction of aromatic spacer groups, useful in production of carbyne-type mol. wires. A two-directional synthesis of a masked hexayne 7, in which two  $\beta$ -chlorovinylsilanes protect two of the internal alkynes, is reported. The key step involves the Pd-catalyzed oxidative dimerization of alkyne HC.tplbond.CC(SiR3):CC(Cl)CH2OTHP (10) to provide diyne THPOCH2CC(Cl)C(SiR3)C.tplbond.CC.tplbond.CC(SiR3):CC(Cl)CH2OTHP (12), which is elaborated into centrosym. masked hexayne 7 in four steps. Masked hexayne 7 is a constitutional isomer of masked hexayne 2, which has been used as a monomer unit for oligoyne assembly. Although masked hexayne 7 was not as convenient a building block as 2 for application in oligoyne assembly, one of its precursors, namely alkyne 10, could be used successfully in Sonogashira couplings, which allowed the incorporation of aromatic spacers and the formation of hybrid masked triyne-phenylenes

Me3SiC.tplbond.CC(Cl)C(SiR3)C.tplbond.C-1,4-C6H4C.tplbond.CC(SiR3):CC(Cl)C.tplbond.CSiMe3 (20) and [Me3SiC.tplbond.CC(Cl)C(SiR3)C.tplbond.C-1,4-C6H4C.tplbond.C]2 (28). Comps. 20 and 28 both contain removable end-groups, which will permit their application as building blocks for the assembly of classes of long-chain,  $\pi$ -conjugated rod-like mol. Rod-like mol.

Me2C(OH)C.tplbond.CC(Cl)C(SiR3)C.tplbond.CC6H4C.tplbond.C)2C(SiR3):CC(Cl)C.tplbond.CCMe2(OH) (34, C6H4 = 1,4-phenylene), which possesses a similar conjugated scaffold as 28, was also prepared by using a similar strategy. Treatment of 34 with TBAF effected a 2-fold dechlorosilylation to provide a rigid rod mol. Me2C(OH)C.tplbond.C)3C6H4C.tplbond.C)2C6H4C.tplbond.C)3CMe2(OH) (35) in which two 1,4-phenylene units interrupt an octayne scaffold.

IT 1191093-44-3F 1191093-45-4P 1191093-46-5P

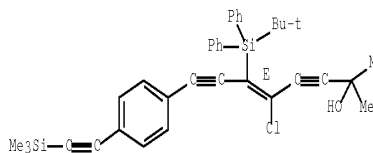
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of  $\pi$ -conjugated p-phenylene-bridged  $\beta$ -chloro silyl-substituted enynes as precursors for arylene-containing polyyne mol. wires)

RN 1191093-44-3 CAPLUS

CN INDEX NAME NOT YET ASSIGNED

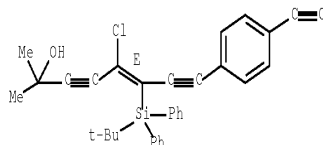
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RN 1191093-45-4 CAPLUS

CN INDEX NAME NOT YET ASSIGNED

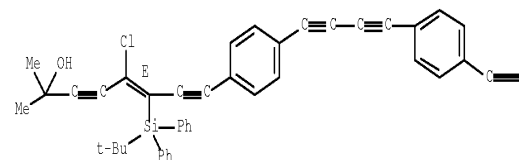
Double bond geometry as shown.



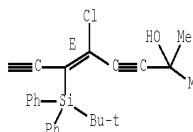
RN 1191093-46-5 CAPLUS

CN 5-Octene-3,7-diyn-2-ol, 8,8'-(1,3-butadiyne-1,4-diyl-di-4,1-phenylene)bis[5-chloro-6-[(1,1-dimethylethyl)diphenylsilyl]-2-methyl-, (5E,5'E)- (CA INDEX NAME)

Double bond geometry as shown.



PAGE 1-A



PAGE 1-B

IT 1191093-44-3P 1191093-45-4P

RL: SPN (Synthetic preparation); PREP (Preparation)

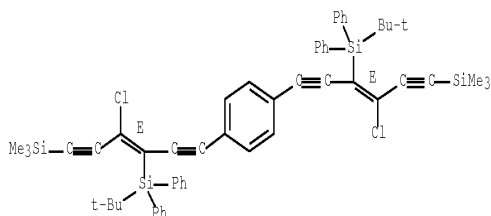


(preparation of  $\pi$ -conjugated p-phenylene-bridged  $\beta$ -chloro silyl-substituted enynes as precursors for arylene-containing polyyne mol. wires)

RN 1191093-33-0 CAPLUS

CN Benzene, 1,4-bis[(3E)-4-chloro-3-[(1,1-dimethylethyl)diphenylsilyl]-6-(trimethylsilyl)-3-hexene-1,5-diyn-1-yl]- (CA INDEX NAME)

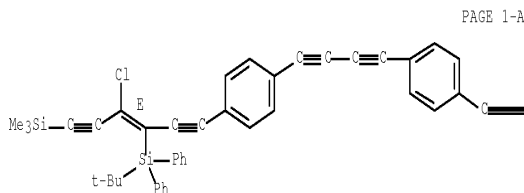
Double bond geometry as shown.



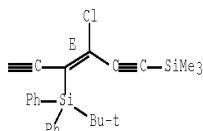
RN 1191093-41-0 CAPLUS

CN Benzene, 1,1'-(1,3-butadiyne-1,4-diyl)bis[4-[(3E)-4-chloro-3-[(1,1-dimethylethyl)diphenylsilyl]-6-(trimethylsilyl)-3-hexene-1,5-diyn-1-yl]- (CA INDEX NAME)

Double bond geometry as shown.



PAGE 1-A



PAGE 1-B

REFERENCE COUNT: 60 THERE ARE 60 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 2 OF 39 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 2009:1099083 CAPLUS Full-text

DOCUMENT NUMBER: 151:508432  
TITLE: Hybrid Conjugated Organic Oligomers Consisting of Oligodiacyetylene and Thiophene Units: Synthesis and Optical Properties

AUTHOR(S): Pilzak, Gregor S.; van Gruijthuijsen, Kitty; van Doorn, Reindert H.; van Lagen, Barend; Sudhoelter, Ernst J. R.; Zuilhof, Han

CORPORATE SOURCE: Laboratory of Organic Chemistry, Wageningen University, Dreijenplein 8, Wageningen, 6703 HB, Neth.

SOURCE: Chemistry--A European Journal (2009), 15(36), 9085-9096, S9085/1-S9085/19

CODEN: CEUJED; ISSN: 0947-6539

PUBLISHER: Wiley-VCH Verlag GmbH & Co. KGaA

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 151:508432

AB Novel and highly soluble hybrid conjugated organic oligomers consisting of oligodiacyetylene and thiophene units have been synthesized in high purity through iterative and divergent approaches based on a sequence of Sonogashira reactions. The series of thiophene-containing oligodiacyetylenes and homocoupled oligodiacyetylenes show, both in solution and in the solid state, a strong optical absorption, which is progressively red shifted with increasing chain length. The linear correlation of the absorption maximum with the inverse of conjugation length (CL = number of double and triple bonds) shows that the effective conjugation length of this system is extended up to at least CL = 20. Furthermore, absorption measurements of dropcast thin films display not only a bathochromic shift of the absorption maxima but also a higher wavelength absorption, which is attributed to increased  $\pi$ - $\pi$  interactions. The wavelength of the maximum fluorescence emission also increases with CL, and emission is maximal for oligomers with CL = 7-12 (fluorescence quantum yield  $\Phi_F$  = .apprx.0.2). Both longer and shorter oligomers display marginal emission. The calculated Stokes shifts of these planar materials are relatively large (0.4 eV) for all oligomers, and likely due to excitation to the S2 state, thus suggesting that the presence of enyne moieties dominates the ordering of the lowest excited states. The fluorescence lifetimes ( $\tau_F$ ) are short ( $\tau_{Fmax}$  = «1 ns) and closely follow the tendency obtained for the fluorescence quantum yield. The anisotropy lifetimes show a near-linear increase with CL in line with highly rigid oligomers.

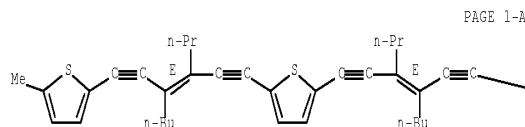
IT 1192220-79-3P 1192220-80-6F 1192220-84-0P  
1192220-86-2P 1192220-90-8P 1192220-92-6P

RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)  
(synthesis via iterative Sonogashira coupling and optical properties of hybrid conjugated organic oligomers consisting of oligodiacyetylene and thiophene units)

RN 1192220-79-3 CAPLUS

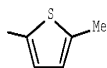
CN INDEX NAME NOT YET ASSIGNED

Double bond geometry as shown.

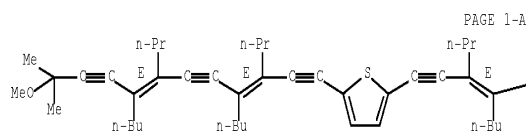


PAGE 1-A



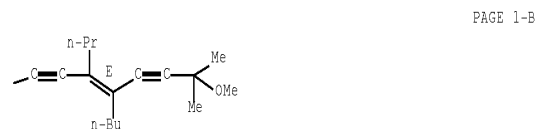
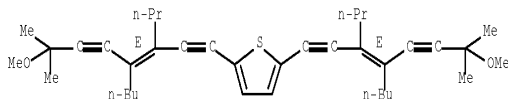


PAGE 1-B



RN 1192820-80-6 CAPLUS  
CN Thiophene, 2,5-bis[(3E)-4-butyl-7-methoxy-7-methyl-3-propyl-3-octene-1,5-diyn-1-yl]- (CA INDEX NAME)

Double bond geometry as shown.

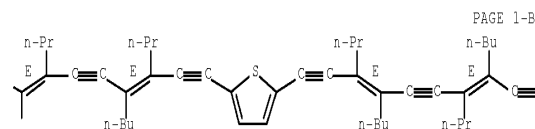
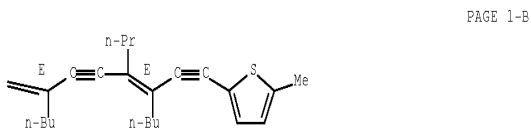
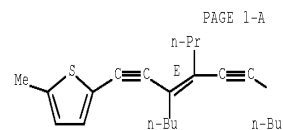
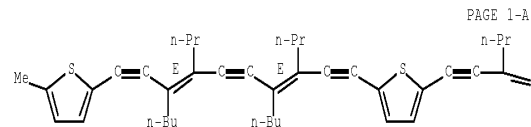


RN 1192820-90-8 CAPLUS  
CN Thiophene, 2,5-bis[(3E,7E,11E)-4,8-dibutyl-12-[2-(5-methyl-2-thienyl)ethynyl]-3,7,11-tripropyl-3,7,11-hexadecatriene-1,5,9-triyn-1-yl]- (CA INDEX NAME)

Double bond geometry as shown.

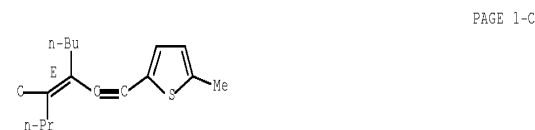
RN 1192820-84-0 CAPLUS  
CN Thiophene, 2,5-bis[(3E,7E)-4-butyl-8-[2-(5-methyl-2-thienyl)ethynyl]-3,7-dipropyl-3,7-dodecadiene-1,5-diyn-1-yl]- (CA INDEX NAME)

Double bond geometry as shown.



RN 1192820-86-2 CAPLUS  
CN INDEX NAME NOT YET ASSIGNED

Double bond geometry as shown.

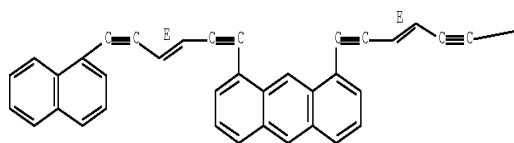
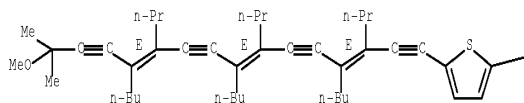


RN 1192820-92-0 CAPLUS

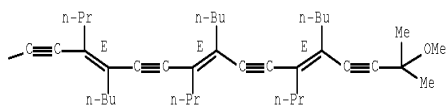


Double bond geometry as shown.

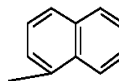
PAGE 1-A



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PAGE 1-B



REFERENCE COUNT: 56 THERE ARE 56 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 3 OF 39 CAPLUS COPYRIGHT 2009 ACS on STN  
 ACCESSION NUMBER: 2007:46877 CAPLUS Full-text  
 DOCUMENT NUMBER: 148:284829  
 TITLE: Synthesis of smallest unit model of graphite intercalation compound and its possibility  
 AUTHOR(S): Ogoshi, Sensuske  
 CORPORATE SOURCE: Department of Applied Chemistry, Faculty of Engineering, Osaka University, Japan  
 SOURCE: Asahi Garasu Zaidan Josei Kenkyu Seika Hokoku (2006) 01.03.07/1-01.03.07/8  
 CODEN: AGSHEN; ISSN: 0919-9179  
 PUBLISHER: Asahi Garasu Zaidan  
 DOCUMENT TYPE: Journal; (computer optical disk)  
 LANGUAGE: Japanese  
 OTHER SOURCE(S): CASREACT 148:284829

AB Graphite is perhaps the simplest layered structure. Many substances can be intercalated between layers of graphite. Upon intercalation, the graphite layers moved apart somewhat due to the intercalated atom. However, the layers still keep parallel each other which would be the key for the formation of intercalation compds. Thus, compds. having two aromatic rings, which can change the distance between the rings and keep parallel to each other, were designed and synthesized. The target compound was 1,8-bis[6-(1-naphthalenyl)-3-hexene-1,5-diynyl]anthracene.

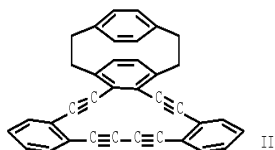
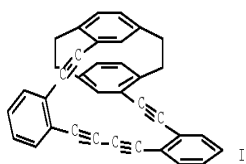
IT 1007602-95-0P  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (preparation of bis[(naphthalenyl)hexenediynyl]anthracene (smallest unit model for graphite intercalation compound))

RN 1007602-95-0 CAPLUS  
 CN Anthracene, 1,8-bis[(3E)-6-(1-naphthalenyl)-3-hexene-1,5-diyn-1-yl]- (CA INDEX NAME)

Double bond geometry as shown.

L8 ANSWER 4 OF 39 CAPLUS COPYRIGHT 2009 ACS on STN  
 ACCESSION NUMBER: 2006:1027761 CAPLUS Full-text  
 DOCUMENT NUMBER: 146:27609  
 TITLE: Phane properties of [2.2]paracyclophane/dehydrobenzoannulene hybrids  
 AUTHOR(S): Hinrichs, Heino; Boydston, Andrew J.; Jones, Peter G.; Hess, Kirsten; Herges, Rainer; Haley, Michael M.; Hopf, Henning  
 CORPORATE SOURCE: Institut fuer Organische Chemie, Technische Universitaet Braunschweig, Braunschweig, 38106, Germany  
 SOURCE: Chemistry--A European Journal (2006), 12(27), 7103-7115  
 CODEN: CEUJED; ISSN: 0947-6539  
 PUBLISHER: Wiley-VCH Verlag GmbH & Co. KGaA  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 OTHER SOURCE(S): CASREACT 146:27609  
 GI





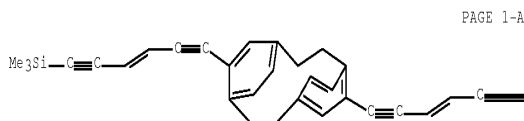
AB Macrocyclic hybrids of [2.2]paracyclophanes with dehydrobenzo[14]annulenes and dehydro[14]annulenes such as I and II are prepared. The UV/visible absorption spectra of the hybrids are compared to determine the communication between the aromatic rings of the paracyclophane units. For some of the title compds. and unsubstituted derivs., the anisotropy of induced c.d. is determined by calcn. to determine the effect of twisting in the perimeter of the macrocycles on the aromaticity of the component structures. The structures of a tetraethynyl[2.2]paracyclophane and of a twisted macrocyclic annulene are determined by X-ray crystallog.

IT 375366-59-9F 865470-27-5P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(preparation and UV/visible absorption spectra of macrocyclic hybrids of [2.2]paracyclophanes with dehydrobenzo[14]annulenes and dehydro[14]annulenes and the anisotropy of induced c.d. and crystal structures of selected compds.)

RN 375366-59-9 CAPLUS

CN Tricyclo[8.2.2.24,7]hexadeca-4,6,10,12,13,15-hexaene, 5,11-bis[6-(trimethylsilyl)-3-hexene-1,5-diyn-1-yl]-, stereoisomer (CA INDEX NAME)

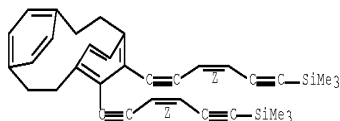


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RN 865470-27-5 CAPLUS  
CN Tricyclo[8.2.2.24,7]hexadeca-4,6,10,12,13,15-hexaene, 5,6-bis[(3Z)-6-(trimethylsilyl)-3-hexene-1,5-diyn-1-yl]- (CA INDEX NAME)

Double bond geometry as shown.



OS.CITING REF COUNT: 13 THERE ARE 13 CAPLUS RECORDS THAT CITE THIS RECORD (13 CITINGS)  
REFERENCE COUNT: 46 THERE ARE 46 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 5 OF 39 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 2005:1004691 CAPLUS Full-text

DOCUMENT NUMBER: 143:306181

TITLE: Process for preparation of  $\pi$ -conjugated aromatic ring-containing acetylene derivatives as organic electroluminescent devices

INVENTOR(S): Sato, Fumie; Takayama, Yuuki

PATENT ASSIGNEE(S): Nissan Chemical Industries, Ltd., Japan

SOURCE: PCT Int. Appl., 82 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

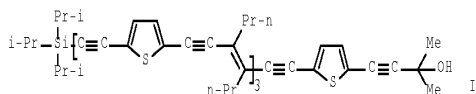
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005085176	A1	20050915	WO 2005-JP3950	20050308
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RW:	BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG			
US 20070176164	A1	20070802	US 2007-591950	20070307
PRIORITY APPLN. INFO.:			JP 2004-65446	A 20040309
			WO 2005-JP3950	W 20050308

ASSIGNMENT HISTORY FOR US PATENT AVAILABLE IN LSUS DISPLAY FORMAT

OTHER SOURCE(S): MARPAT 143:306181

GI





AB This invention pertains to a method for producing  $\pi$ -conjugated aromatic ring-containing acetylene derivs. via coupling reaction in the presence of palladium and Cu(I) catalysts. For example, the compound I was prepared in a multi-step synthesis in good yield. The title compds. are useful as electroluminescent devices.

IT 740810-64-4P 740810-65-5P 740810-67-7P  
740810-68-8P 864683-96-5P 864683-97-6P  
864684-01-5P 864684-02-6P 864684-04-8P  
864684-05-9P 864684-31-1P 864684-32-2P

RL: IMF (Industrial manufacture); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(intermediate; preparation of  $\pi$ -conjugated aromatic ring-containing acetylene derivs. as organic electroluminescent devices)

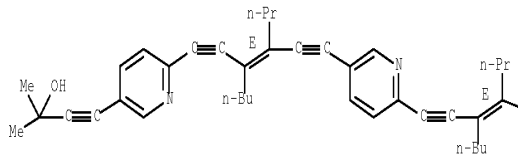
RN 740810-64-4 CAPLUS

CN 3-Butyn-2-ol, 4-[6-[(3E)-3-butyl-4-[2-[6-[2-[tris(1-methylethyl)silyl]ethynyl]-3-pyridinyl]ethynyl]-3-hepten-1-yn-1-yl]-3-pyridinyl]-2-methyl- (CA INDEX NAME)

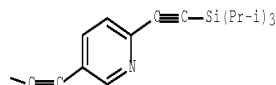
Double bond geometry as shown.

Double bond geometry as shown.

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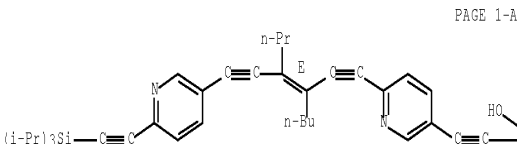
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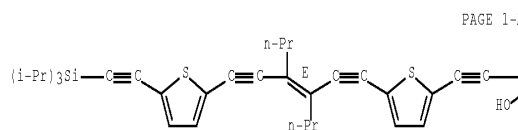
RN 740810-67-7 CAPLUS

CN 3-Butyn-2-ol, 2-methyl-4-[5-[(3E)-3-propyl-4-[5-[tris(1-methylethyl)silyl]ethynyl]-2-thienyl]ethynyl]-3-hepten-1-yn-1-yl]-2-thienyl- (CA INDEX NAME)

Double bond geometry as shown.



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RN 740810-65-5 CAPLUS

CN 3-Butyn-2-ol, 4-[6-[(3E)-3-butyl-4-[2-[6-[(3E)-3-butyl-4-[2-[6-[2-[tris(1-methylethyl)silyl]ethynyl]-3-pyridinyl]ethynyl]-3-hepten-1-yn-1-yl]-3-pyridinyl]ethynyl]-3-hepten-1-yn-1-yl]-3-pyridinyl]-2-methyl- (CA INDEX NAME)



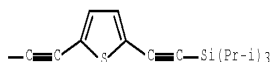
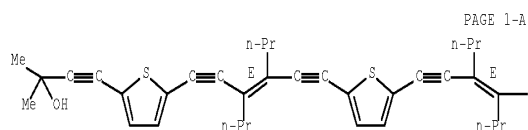
PAGE 1-B

RN 740810-68-8 CAPLUS

CN 3-Butyn-2-ol, 2-methyl-4-[5-[(3E)-3-propyl-4-[5-[tris(1-methylethyl)silyl]ethynyl]-2-thienyl]ethynyl]-3-hepten-1-yn-1-yl]-2-thienyl- (CA INDEX NAME)

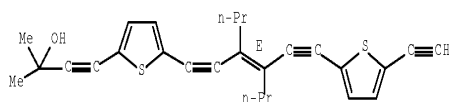
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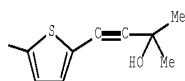
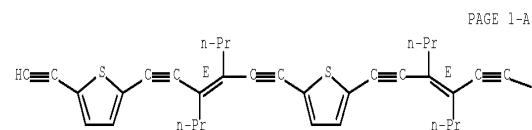
RN 864683-96-5 CAPLUS  
 CN 3-Butyn-2-ol, 4-[5-[(3E)-5-ethyl-4-[2-(5-ethynyl-2-thienyl)ethynyl]-3-propyl-3-penten-1-yn-1-yl]-2-thienyl]-2-methyl- (CA INDEX NAME)

Double bond geometry as shown.



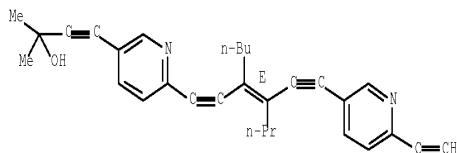
RN 864683-97-6 CAPLUS  
 CN 3-Butyn-2-ol, 4-[5-[(3E)-4-[2-[5-[(3E)-4-[2-(5-ethynyl-2-thienyl)ethynyl]-3-propyl-3-hepten-1-yn-1-yl]-2-thienyl]ethynyl]-3-propyl-3-hepten-1-yn-1-yl]-2-thienyl]-2-methyl- (CA INDEX NAME)

Double bond geometry as shown.



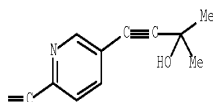
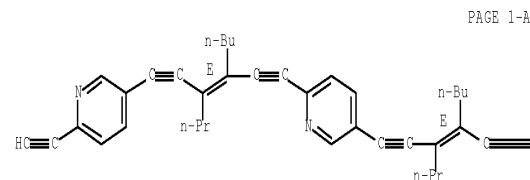
RN 864684-01-5 CAPLUS  
 CN 3-Butyn-2-ol, 4-[6-[(3E)-3-butyl-4-[2-(6-ethynyl-3-pyridinyl)ethynyl]-3-hepten-1-yn-1-yl]-3-pyridinyl]-2-methyl- (CA INDEX NAME)

Double bond geometry as shown.



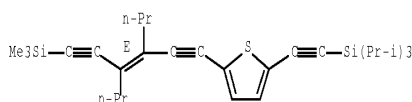
RN 864684-02-6 CAPLUS  
 CN 3-Butyn-2-ol, 4-[6-[(3E)-3-butyl-4-[2-[6-[(3E)-3-butyl-4-[2-(6-ethynyl-3-pyridinyl)ethynyl]-3-hepten-1-yn-1-yl]-3-pyridinyl]ethynyl]-3-hepten-1-yn-1-yl]-3-pyridinyl]-2-methyl- (CA INDEX NAME)

Double bond geometry as shown.



RN 864684-04-8 CAPLUS  
 CN Thiophene, 2-[(3E)-3,4-dipropyl-6-(trimethylsilyl)-3-hexene-1,5-diyn-1-yl]-5-[2-[tris(1-methylethyl)silyl]ethynyl]- (CA INDEX NAME)

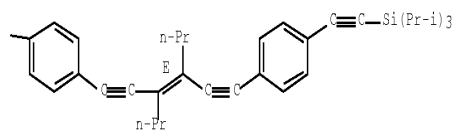
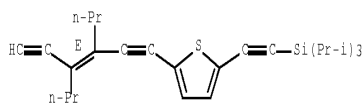
Double bond geometry as shown.





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Double bond geometry as shown.

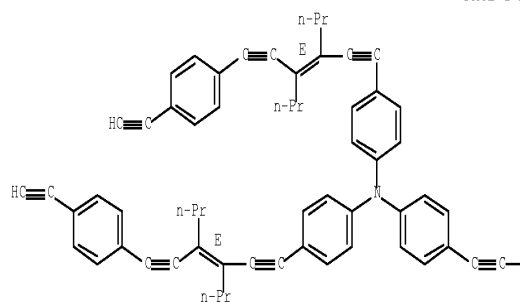
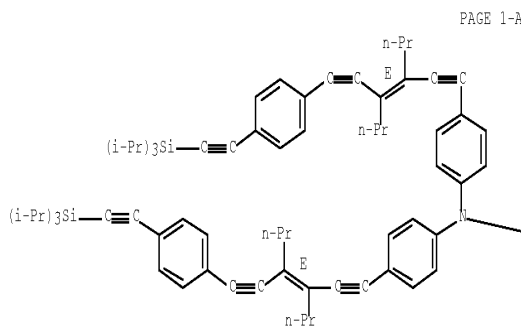


CN Benzenamine, N-[4-[(3E)-3,4-dipropyl-6-[4-[2-[tris(1-methylethyl)silyl]ethynyl]phenyl]-3-hexene-1,5-diyn-1-yl]phenyl]-4-[(3E)-3-propyl-4-[2-[4-[2-[tris(1-methylethyl)silyl]ethynyl]phenyl]ethynyl]-3-hepten-1-yn-1-yl]N-[4-[(3E)-3-propyl-4-[2-[4-[2-[tris(1-methylethyl)silyl]ethynyl]phenyl]ethynyl]-3-hepten-1-yn-1-yl]phenyl]- (CA INDEX NAME)

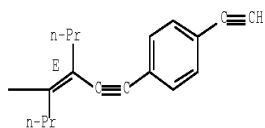
CN Benzenamine, N-[4-[(3E)-5-ethyl-4-[2-(4-ethynylphenyl)ethynyl]-3-propyl-3-penten-1-yn-1-yl]phenyl]-4-[(3E)-4-[2-(4-ethynylphenyl)ethynyl]-3-propyl-3-hepten-1-yn-1-yl]-N-[4-[(3E)-4-[2-(4-ethynylphenyl)ethynyl]-3-propyl-3-hepten-1-yn-1-yl]phenyl]- (CA INDEX NAME)

Double bond geometry as shown.

Double bond geometry as shown.







IT 740810-66-6P 740810-68-8P 864684-03-7P  
 864684-06-0P 864684-09-3P 864684-21-3P  
 864684-22-3P 864684-23-1P 864684-24-2P  
 864684-25-3P 864684-26-4P 864684-27-5P  
 864684-28-6P 864684-29-7P 864684-30-0P  
 864684-33-3P

RL: DEV (Device component use); IMF (Industrial manufacture); SPN  
 (Synthetic preparation); TEM (Technical or engineered material use); PREP  
 (Preparation); USES (Uses)

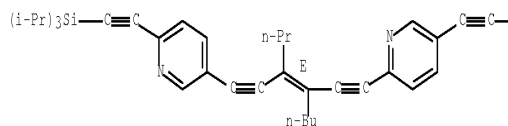
(preparation of  $\pi$ -conjugated aromatic ring-containing acetylene derivs. as  
 organic electroluminescent devices)

RN 740810-66-6 CAPLUS

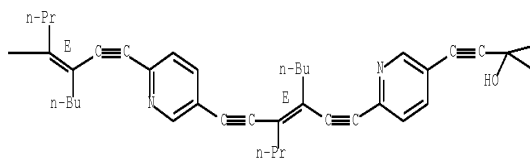
CN 3-Butyn-2-ol, 4-[6-[(3E)-3-butyl-4-[2-[6-[(3E)-3-butyl-4-[2-[6-[(3E)-3-butyl-4-[2-[6-[2-[tris(1-methylethyl)silyl]ethynyl]-3-pyridinyl]ethynyl]-3-hepten-1-yn-1-yl]-3-pyridinyl]ethynyl]-3-hepten-1-yn-1-yl]-3-pyridinyl]ethynyl]-3-hepten-1-yn-1-yl]-3-pyridinyl]-2-methyl- (CA INDEX NAME)

Double bond geometry as shown.

PAGE 1-A



PAGE 1-B



PAGE 1-C

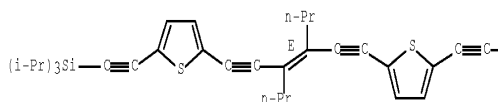


RN 740810-69-9 CAPLUS

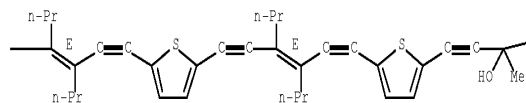
CN 3-Butyn-2-ol, 4-[5-[(3E)-4-[2-[5-[(3E)-5-ethyl-4-[2-[5-[(3E)-5-ethyl-3-propyl-4-[2-[5-[2-[tris(1-methylethyl)silyl]ethynyl]-2-thienyl]ethynyl]-3-penten-1-yn-1-yl]-2-thienyl]ethynyl]-3-propyl-3-penten-1-yn-1-yl]-2-thienyl]ethynyl]-3-propyl-3-hepten-1-yn-1-yl]-2-thienyl]-2-methyl- (CA INDEX NAME)

Double bond geometry as shown.

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PAGE 1-B



PAGE 1-C



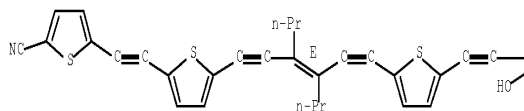
RN 864684-03-7 CAPLUS

CN 2-Thiophenecarbonitrile, 5-[2-[5-[(3E)-5-ethyl-4-[2-[5-(3-hydroxy-3-methyl-1-butyn-1-yl)-2-thienyl]ethynyl]-3-propyl-3-penten-1-yn-1-yl]-2-thienyl]ethynyl]- (CA INDEX NAME)

Double bond geometry as shown.



PAGE 1-A



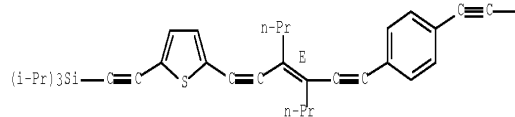
RN 864684-21-9 CAPLUS

CN Thiophene, 2-[(3E)-3,4-dipropyl-6-[4-[(3E)-3-propyl-4-[2-[5-[2-[tris(1-methylethyl)silyl]ethynyl]-2-thienyl]ethynyl]-3-hepten-1-yn-1-yl]phenyl]-3-hexene-1,5-diyn-1-yl]-5-[2-[tris(1-methylethyl)silyl]ethynyl]-

Double bond geometry as shown.

PAGE 1-A

PAGE 1-B

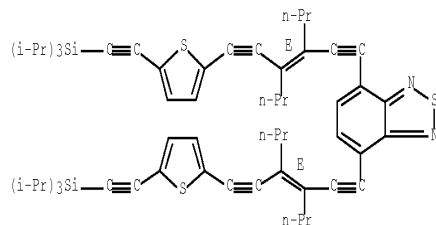
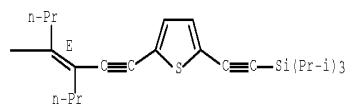


RN 864684-06-0 CAPLUS

CN 2,1,3-Benzothiadiazole, 4-[(3E)-3,4-dipropyl-6-[5-[2-[tris(1-methylethyl)silyl]ethynyl]-2-thienyl]-3-hexene-1,5-diyn-1-yl]-7-[(3E)-3-propyl-4-[2-[5-[2-[tris(1-methylethyl)silyl]ethynyl]-2-thienyl]ethynyl]-3-hepten-1-yn-1-yl]-

Double bond geometry as shown.

PAGE 1-B



RN 864684-22-0 CAPLUS

CN Benzene, 1-[(3E)-3,4-dipropyl-6-[4-[2-[tris(1-methylethyl)silyl]ethynyl]phenyl]-3-hexene-1,5-diyn-1-yl]-4-[(3E)-3-propyl-4-[2-[4-[2-[tris(1-methylethyl)silyl]ethynyl]phenyl]ethynyl]-3-hepten-1-yn-1-yl]-

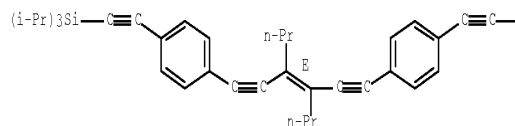
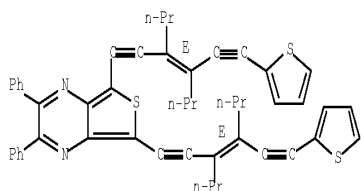
Double bond geometry as shown.

PAGE 1-A

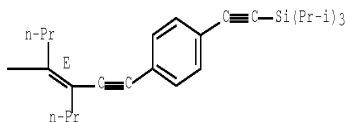
RN 864684-09-3 CAPLUS

CN Thieno[3,4-b]pyrazine, 5-[(3E)-3,4-dipropyl-6-(2-thienyl)-3-hexene-1,5-diyn-1-yl]-2,3-diphenyl-7-[(3E)-3-propyl-4-[2-(2-thienyl)ethynyl]-3-hepten-1-yn-1-yl]-

Double bond geometry as shown.



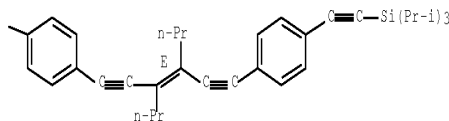
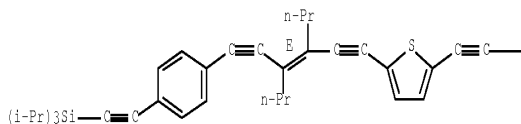




RN 864684-23-1 CAPLUS

CN Thiophene, 2-[(3E)-3,4-dipropyl-6-[4-[2-[tris(1-methylethyl)silyl]ethynyl]phenyl]-3-hexene-1,5-diyn-1-yl]-5-[(3E)-3-propyl-4-[2-[4-[2-[tris(1-methylethyl)silyl]ethynyl]phenyl]ethynyl]-3-hepten-1-yn-1-yl]- (CA INDEX NAME)

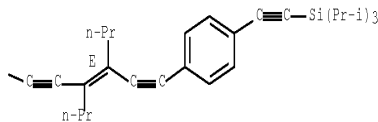
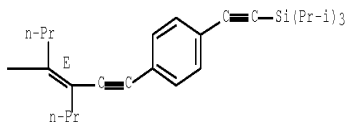
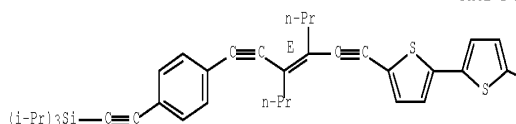
Double bond geometry as shown.



RN 864684-25-3 CAPLUS

CN 2,2'-Bithiophene, 5-[(3E)-3,4-dipropyl-6-[4-[2-[tris(1-methylethyl)silyl]ethynyl]phenyl]-3-hexene-1,5-diyn-1-yl]-5'-[(3E)-3-propyl-4-[2-[4-[2-[tris(1-methylethyl)silyl]ethynyl]phenyl]ethynyl]-3-hepten-1-yn-1-yl]- (CA INDEX NAME)

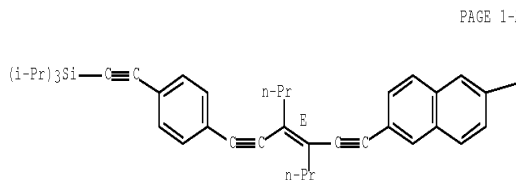
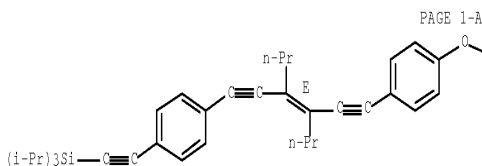
Double bond geometry as shown.



RN 864684-24-2 CAPLUS

CN Silane, [oxybis[4,1-phenylene[(3E)-3,4-dipropyl-3-hexene-1,5-diyne-6,1-diyl]-4,1-phenylene-2,1-ethynediyl]]bis[tris(1-methylethyl)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



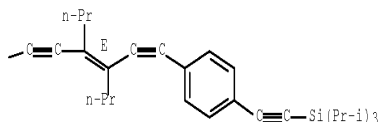
RN 864684-26-4 CAPLUS

CN Naphthalene, 2-[(3E)-3,4-dipropyl-6-[4-[2-[tris(1-methylethyl)silyl]ethynyl]phenyl]-3-hexene-1,5-diyn-1-yl]-6-[(3E)-3-propyl-4-[2-[4-[2-[tris(1-methylethyl)silyl]ethynyl]phenyl]ethynyl]-3-hepten-1-yn-1-yl]- (CA INDEX NAME)

Double bond geometry as shown.



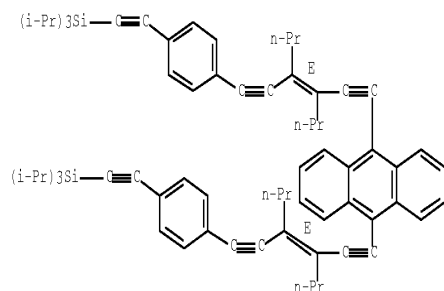
PAGE 1-B



RN 864684-27-5 CAPLUS

CN Anthracene, 9-[(3E)-3,4-dipropyl-6-[4-[2-[tris(1-methylethyl)silyl]ethynyl]phenyl]-3-hexene-1,5-diyn-1-yl]-10-[(3E)-3-propyl-4-[2-[4-[2-[tris(1-methylethyl)silyl]ethynyl]phenyl]ethynyl]-3-hepten-1-yn-1-yl]- (CA INDEX NAME)

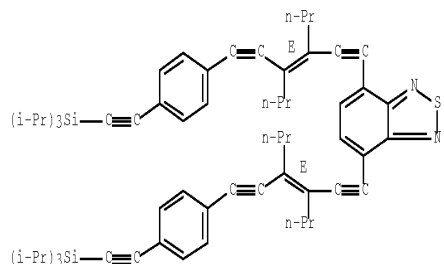
Double bond geometry as shown.



RN 864684-28-6 CAPLUS

CN 2,1,3-Benzothiadiazole, 4-[(3E)-3,4-dipropyl-6-[4-[2-[tris(1-methylethyl)silyl]ethynyl]phenyl]-3-hexene-1,5-diyn-1-yl]-7-[(3E)-3-propyl-4-[2-[4-[2-[tris(1-methylethyl)silyl]ethynyl]phenyl]ethynyl]-3-hepten-1-yn-1-yl]- (CA INDEX NAME)

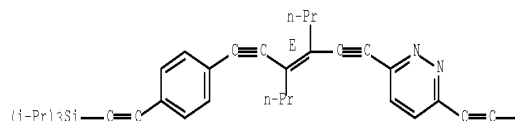
Double bond geometry as shown.



RN 864684-29-7 CAPLUS

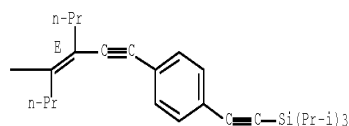
CN Pyridazine, 3-[(3E)-3,4-dipropyl-6-[4-[2-[tris(1-methylethyl)silyl]ethynyl]phenyl]-3-hexene-1,5-diyn-1-yl]-6-[(3E)-3-propyl-4-[2-[4-[2-[tris(1-methylethyl)silyl]ethynyl]phenyl]ethynyl]-3-hepten-1-yn-1-yl]- (CA INDEX NAME)

Double bond geometry as shown.



PAGE 1-A

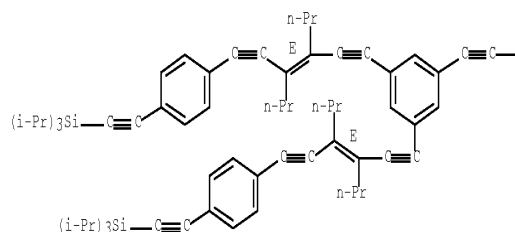
PAGE 1-B



RN 864684-30-0 CAPLUS

CN Benzene, 1-[(3E)-3,4-dipropyl-6-[4-[2-[tris(1-methylethyl)silyl]ethynyl]phenyl]-3-hexene-1,5-diyn-1-yl]-3-[(3E)-5-ethyl-3-propyl-4-[2-[4-[2-[tris(1-methylethyl)silyl]ethynyl]phenyl]ethynyl]-3-penten-1-yn-1-yl]-5-[(3E)-3-propyl-4-[2-[4-[2-[tris(1-methylethyl)silyl]ethynyl]phenyl]ethynyl]-3-hepten-1-yn-1-yl]- (CA INDEX NAME)

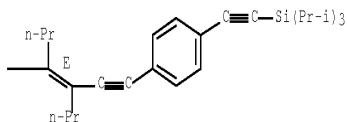
Double bond geometry as shown.



PAGE 1-A



PAGE 1-B

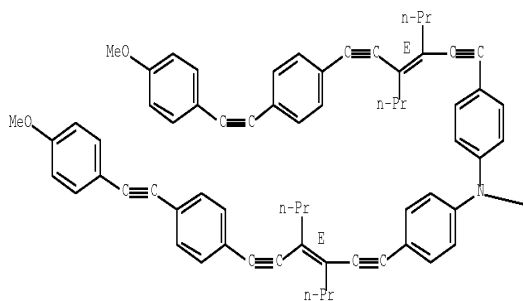


RN 864684-33-3 CAPLUS

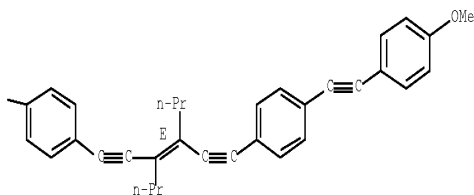
CN Benzenamine, N-[4-[(3E)-5-ethyl-4-[2-[4-[2-(4-methoxyphenyl)ethynyl]phenyl]ethynyl]-3-propyl-3-penten-1-yn-1-yl]phenyl]-4-[(3E)-4-[2-[4-[2-(4-methoxyphenyl)ethynyl]phenyl]ethynyl]-3-propyl-3-hepten-1-yn-1-yl]-N-[4-[(3E)-4-[2-[4-[2-(4-methoxyphenyl)ethynyl]phenyl]ethynyl]-3-propyl-3-hepten-1-yn-1-yl]phenyl]- (CA INDEX NAME)

Double bond geometry as shown.

PAGE 1-A



PAGE 1-B



REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS

L8 ANSWER 6 OF 39 CAPLUS COPYRIGHT 2009 ACS ON STN

ACCESSION NUMBER: 2005:630411 CAPLUS [Full-text](#)

DOCUMENT NUMBER: 143:346727

TITLE: [2.2]Paracyclophane/Dehydroannulene Hybrids: Probing the Aromaticity of the Dehydro[14]annulene Framework  
 AUTHOR(S): Hinrichs, Heino; Fischer, Axel K.; Jones, Peter G.; Hopf, Henning; Haley, Michael M.

CORPORATE SOURCE: Department of Chemistry, University of Oregon, Eugene, OR, 97403-1253, USA

SOURCE: Organic Letters (2005), 7(17), 3793-3795  
 CODEN: ORLEF7; ISSN: 1523-7060

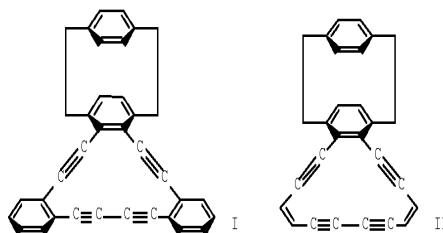
PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 143:346727

GI



AB The synthesis of [2.2]paracyclophane/dehydro[14]annulene hybrids I and II is reported. Comparison of the proton NMR spectra of I and II with their open precursors and with related model compds. reveals the pronounced effect of macrocycle formation upon the cyclophane protons H15/H16, which lie above the shielding cone of the diatropic [14]annulene moiety.

IT 865470-27-5P

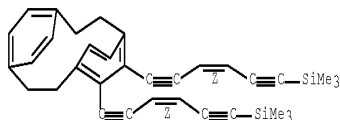
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(paracyclophane dehydroannulene hybrids probing aromaticity of dehydroannulene framework)

RN 865470-27-5 CAPLUS

CN Tricyclo[8.2.2.24,7]hexadeca-4,6,10,12,13,15-hexaene, 5,6-bis[(3Z)-6-(trimethylsilyl)-3-hexene-1,5-diyn-1-yl]- (CA INDEX NAME)

Double bond geometry as shown.





OS.CITING REF COUNT: 8 THERE ARE 8 CAPLUS RECORDS THAT CITE THIS RECORD (8 CITINGS)

REFERENCE COUNT: 22 THERE ARE 22 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 7 OF 39 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 2005:354187 CAPLUS [Full-text](#)

DOCUMENT NUMBER: 143:333

TITLE: Cytotoxicities, cell cycle and caspase evaluations of 1,6-diaryl-3(Z)-hexen-1,5-diyne, 2-(6-aryl-3(Z)-hexen-1,5-diynyl)anilines and their derivatives

AUTHOR(S): Lin, Chi-Fong; Lo, Yu-Hsiang; Hsieh, Ming-Chu; Chen, Yi-Hua; Wang, Jeh-Jeng; Wu, Ming-Jung

CORPORATE SOURCE: School of Chemistry, Kaohsiung Medical University, Kaohsiung, Taiwan

SOURCE: Bioorganic & Medicinal Chemistry (2005), 13(10), 3565-3575

CODEN: BMECEP; ISSN: 0968-0896

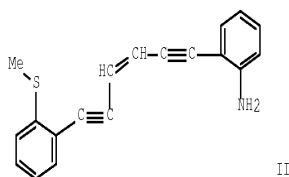
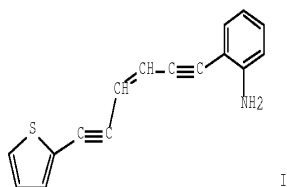
PUBLISHER: Elsevier Ltd.

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 143:333

GI



AB A series of compds. showed growth inhibition effects on a full panel of 60 human cancer cell lines, and most of the average IC50 values of the indicated analogs were from <0.01 to 96.6  $\mu$ M, in which a 2-thienyl analog and the thioanisole analog revealed the highest cytotoxic activity with the cancer cell lines at 10-7M concentration range. During the cell cycle anal., a moderate to high apoptotic progress induction was shown by several compared with the control, which 2-(6-(2-thienyl)-3(Z)-hexen-1,5-diynyl)aniline (I) showed the highest apoptotic effect. I and the thioanisole analog displayed a significant G2/M phase arrest in the cell growth cycle compared with other derivs., which the proportions of the G2/M phase cells were accumulated to 71.5% and 82.6%, resp. Moreover, the colorimetric assay of the I and the thioanisole analog also provided advanced evidence to the relationship between

the compds. and the caspase-3 enzyme, which was one of the major promoters of apoptotic effect.

IT #52619-13-7P

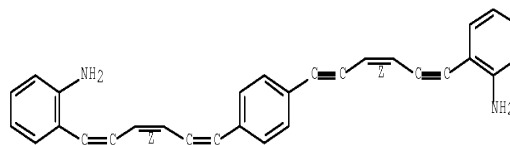
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)

(cytotoxicities, cell cycle and caspase evaluations of 1,6-diaryl-3(Z)-hexen-1,5-diyne, 2-(6-aryl-3(Z)-hexen-1,5-diynyl)anilines and their derivs.)

RN 852619-13-7 CAPLUS

CN Benzenamine, 2,2'-[1,4-phenylenedi-(3Z)-3-hexene-1,5-diyne-6,1-diyl]bis-(9CI) (CA INDEX NAME)

Double bond geometry as shown.



OS.CITING REF COUNT: 15 THERE ARE 15 CAPLUS RECORDS THAT CITE THIS RECORD (15 CITINGS)

REFERENCE COUNT: 35 THERE ARE 35 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 8 OF 39 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 2005:17022 CAPLUS [Full-text](#)

DOCUMENT NUMBER: 142:113747

TITLE: Preparation of aryl-substituted acyclic enediyne compounds as antitumor agents

INVENTOR(S): Wu, Ming-Jung; Lin, Chi-Fong

PATENT ASSIGNEE(S): Kaohsiung Medical University, Taiwan

SOURCE: U.S. Pat. Appl. Publ., 41 pp.

CODEN: USXXCO

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 2

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 20050004212	A1	20050106	US 2004-847667	20040518
US 7332623	B2	20080219		
CA 2570366	A1	20050317	CA 2004-2570366	20040909
WO 2005023131	A2	20050317	WO 2004-US29334	20040909
WO 2005023131	A3	20050512		

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SN, TD, TG

WO 2005023146 A2 20050317 WO 2004-US29338 20040909

WO 2005023146 A3 20050512

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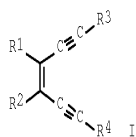
US 2006-488204 A1 20060718

ASSIGNMENT HISTORY FOR US PATENT AVAILABLE IN LSUS DISPLAY FORMAT

OTHER SOURCE(S): MARPAT 142:113747

GI





Q=



Q1=



AB This invention provides aryl-substituted acyclic enediyne compds. of formula (I) or pharmaceutically acceptable salts or solvates thereof (wherein R1 = R2 = H; or R1 and R2 together form a moiety represented by the formula Q or Q1; R3 = (un)substituted C4-30 alkyl or C3-30 aryl; R4 = (un)substituted C3-30 aryl; with the proviso that R3 is not Bu, pentyl, tetrahydropyranyloxymethyl, tetrahydropyranyloxypropyl or Ph when R1 = R2 = H and R4 = o-cyanophenyl; and with the proviso that R3 is not Bu when R1 = R2 = H and R4 = Ph). These compds. found to have inhibitory activities against topoisomerase I or act as a S phase or G2/M phase blocker and were also tested in vitro in anticancer assay. 4-((Z)-3-Dodecen-1,5-diynyl)-1-trifluoromethylbenzene and 2-((Z)-3-dodecen-1,5-diynyl)pyrazine showed IC50 of 4.32 and 5.93 µg/mL against human solid tumor KB cells.

IT 457314-65-7P

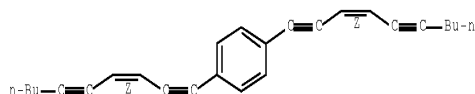
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of aryl-substituted acyclic enediyne compds. as antitumor agents, topoisomerase I inhibitors, or S phase or G2/M phase blockers)

RN 457914-65-7 CAPLUS

CN Benzene, 1,4-di(3Z)-3-decene-1,5-diyn-1-yl- (CA INDEX NAME)

Double bond geometry as shown.



REFERENCE COUNT: 39 THERE ARE 39 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 9 OF 39 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 2005:15944 CAPLUS [Full-text](#)

DOCUMENT NUMBER: 142:113746

TITLE: Preparation of aryl-substituted acyclic enediyne compounds as antitumor agents and pharmaceutical compositions comprising them

INVENTOR(S): Wu, Ming-Jung; Lin, Chi-Fong

PATENT ASSIGNEE(S): Kaohsiung Medical University, Taiwan

SOURCE: U.S. Pat. Appl. Publ., 41 pp.  
CODEN: USXXCO

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 2

PATENT INFORMATION:

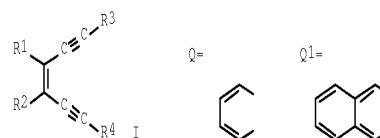
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CA 2570366	A1	20050317	CA 2004-2570366	20040909
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OTHER SOURCE(S): MARPAT 142:113746  
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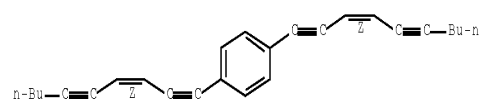


AB A pharmaceutical compns. comprises aryl-substituted acyclic enediyne compds. of formula (I) or pharmaceutically acceptable salts thereof (wherein R1 = R2 = H; or R1 and R2 together form a moiety represented by the formula Q or Q1; R3 = (un)substituted C4-30 alkyl or C3-30 aryl; R4 = (un)substituted C3-30 aryl; with the proviso that R3 is not Bu, pentyl, tetrahydropyranyloxymethyl, tetrahydropyranyloxypropyl or Ph when R1 = R2 = H and R4 = o-cyanophenyl; and with the proviso that R3 is not Bu when R1 = R2 = H and R4 = Ph). The pharmaceutical composition is used to treat a subject afflicted with a tumor/cancer by inhibiting topoisomerase I activities or blocking the S phase or G2/M phase of the tumor/cancer cells. The tumor/cancer cell is selected from leukemia cancer cells, non-small-cell lung cancer cells, col on cancer cells, CNS cancer cells, melanoma cancer cells, ovarian cancer cells, renal cancer cells, prostate cancer cells and breast cancer cells. These compds. were tested in vitro for inhibitory activities against topoisomerase I, cell cycle at a S phase or G2/M phase blocker, and anticancer growth. For example, 4-((Z)-3-Dodecen-1,5-diynyl)-1-trifluoromethylbenzene and 2-((Z)-3-dodecen-1,5-diynyl)pyrazine showed IC50 of 4.32 and 5.93 µg/mL against human solid tumor KB cells.

IT 457914-65-7P  
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)  
(preparation of aryl-substituted acyclic enediyne compds. as antitumor agents, topoisomerase I inhibitors, or S phase or G2/M phase blockers)

RN 457914-65-7 CAPLUS  
CN Benzene, 1,4-di(3Z)-3-decene-1,5-diyn-1-yl- (CA INDEX NAME)

Double bond geometry as shown.



OS.CITING REF COUNT: 3 THERE ARE 3 CAPLUS RECORDS THAT CITE THIS RECORD (4 CITINGS)

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L8 ANSWER 10 OF 39 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 2004:480115 CAPLUS Full-text

DOCUMENT NUMBER: 141:190674

TITLE: Synthesis of Conjugated Oligomers Having Aromatic and Enediyne Units Alternately in the Backbone that Show Intense Fluorescence Emission

PAGE 1-B

AUTHOR(S): Nakano, Yuuki; Ishizuka, Kenichi; Muraoka, Kenji; Ohtani, Hiroyuki; Takayama, Yuuki; Sato, Fumie

CORPORATE SOURCE: Department of Biomolecular Engineering, Tokyo Institute of Technology, Midori, Yokohama, Kanagawa, 226-8501, Japan

SOURCE: Organic Letters (2004), 6(14), 2373-2376

CODEN: ORLEF7; ISSN: 1523-7060

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 141:190674

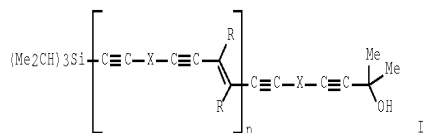
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RN 740810-62-2 CAPLUS

CN 3-Butyn-2-ol, 2-methyl-4-[4-[(3E)-3-propyl-4-[[4-[(3E)-3-propyl-4-[[4-[[tris(1-methylethyl)silyl]ethynyl]phenyl]ethynyl]-3-hepten-1-yn-1-yl]phenyl]ethynyl]-3-hepten-1-yn-1-yl]phenyl]- (CA INDEX NAME)

Double bond geometry as shown.



AB Synthesis and fluorescence properties of  $\pi$ -conjugated compds. I ( $n = 1 - 3$ ; X = 1,4-phenylene, 2,5-pyridine, 2,5-thiophene; R = n-Pr, n-Bu) having alternately an aromatic or heteroarom. ring and an enediyne unit in the backbone are described.

PAGE 1-B

IT 740810-61-1P 740810-62-2P 740810-64-4P

740810-65-5P 740810-67-7P 740810-68-8P

RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

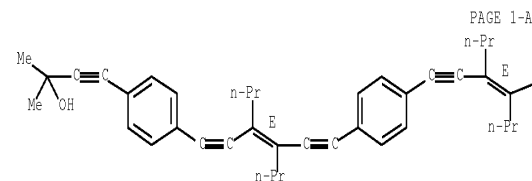
(preparation and absorption and fluorescence spectra of conjugated oligomers

having aromatic (or heteroarom.) and enediyne units alternately in the backbone)

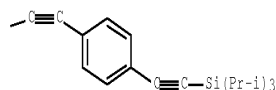
RN 740810-61-1 CAPLUS

CN 3-Butyn-2-ol, 2-methyl-4-[4-[(3E)-3-propyl-4-[2-[4-[2-[tris(1-methylethyl)silyl]ethynyl]phenyl]ethynyl]-3-hepten-1-yn-1-yl]phenyl]- (CA INDEX NAME)

Double bond geometry as shown.



PAGE 1-A

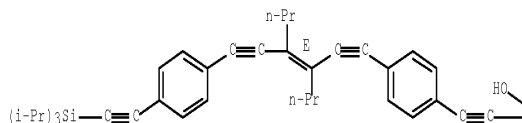


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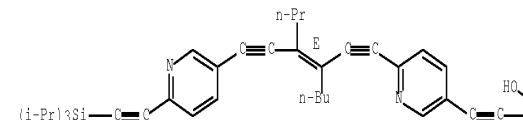
CN 3-Butyn-2-ol, 4-[6-[(3E)-3-butyl-4-[2-[6-[2-[tris(1-methylethyl)silyl]ethynyl]-3-pyridinyl]ethynyl]-3-hepten-1-yn-1-yl]-3-pyridinyl]-2-methyl- (CA INDEX NAME)

Double bond geometry as shown.

PAGE 1-A



PAGE 1-A





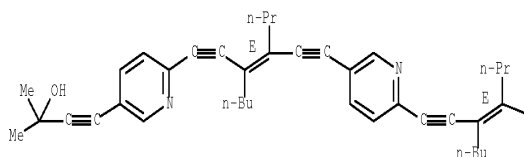


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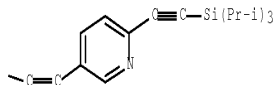
CN 3-Butyn-2-ol, 4-[6-[(3E)-3-butyl-4-[2-[6-[(3E)-3-butyl-4-[2-[6-[2-[tris(1-methylethyl)silyl]ethynyl]-3-pyridinyl]ethynyl]-3-hepten-1-yn-1-yl]-3-pyridinyl]ethynyl]-3-hepten-1-yn-1-yl]-3-pyridinyl]-2-methyl- (CA INDEX NAME)

Double bond geometry as shown.

PAGE 1-A



PAGE 1-B

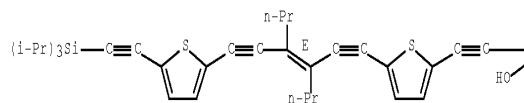


RN 740810-67-7 CAPLUS

CN 3-Butyn-2-ol, 2-methyl-4-[5-[(3E)-3-propyl-4-[[5-[[tris(1-methylethyl)silyl]ethynyl]-2-thienyl]ethynyl]-3-hepten-1-yn-1-yl]-2-thienyl]- (CA INDEX NAME)

Double bond geometry as shown.

PAGE 1-A

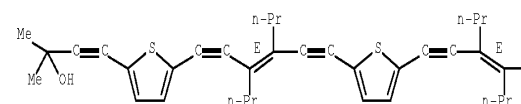


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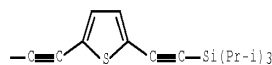
CN 3-Butyn-2-ol, 2-methyl-4-[5-[(3E)-3-propyl-4-[[5-[[tris(1-methylethyl)silyl]ethynyl]-2-thienyl]ethynyl]-3-hepten-1-yn-1-yl]-2-thienyl]ethynyl]-3-hepten-1-yn-1-yl]-2-thienyl]- (CA INDEX NAME)

Double bond geometry as shown.

PAGE 1-A



PAGE 1-B



IT 740810-63-3P 740810-66-6P 740810-63-3P

RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)  
(preparation and absorption and fluorescence spectra of conjugated

oligomers

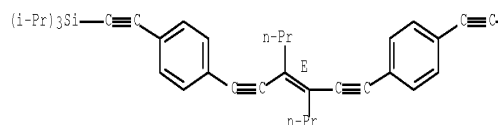
having aromatic (or heteroarom.) and enediyne units alternately in the backbone)

RN 740810-63-3 CAPLUS

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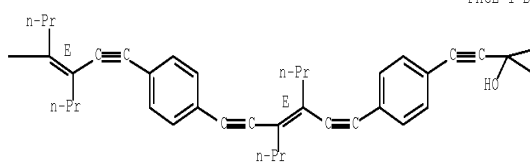
Double bond geometry as shown.

PAGE 1-A





PAGE 1-C



PAGE 1-B



RN 740810-69-9 CAPLUS

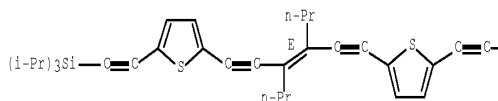
CN 3-Butyn-2-ol, 4-[5-[(3E)-4-[2-[5-[(3E)-5-ethyl-4-[2-[5-[(3E)-5-ethyl-3-propyl-4-[2-[5-[2-[tris(1-methylethyl)silyl]ethynyl]-2-thienyl]ethynyl]-3-penten-1-yn-1-yl]-2-thienyl]ethynyl]-3-propyl-3-penten-1-yn-1-yl]-2-thienyl]ethynyl]-3-propyl-3-hepten-1-yn-1-yl]-2-thienyl]-2-methyl- (CA INDEX NAME)

Double bond geometry as shown.

PAGE 1-C



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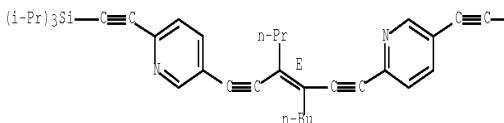


RN 740810-66-6 CAPLUS

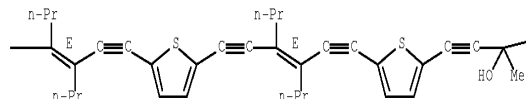
CN 3-Butyn-2-ol, 4-[6-[(3E)-3-butyl-4-[2-[6-[(3E)-3-butyl-4-[2-[6-[(3E)-3-butyl-4-[2-[6-[2-[tris(1-methylethyl)silyl]ethynyl]-3-pyridinyl]ethynyl]-3-hepten-1-yn-1-yl]-3-pyridinyl]ethynyl]-3-hepten-1-yn-1-yl]-3-pyridinyl]ethynyl]-3-hepten-1-yn-1-yl]-3-pyridinyl]-2-methyl- (CA INDEX NAME)

Double bond geometry as shown.

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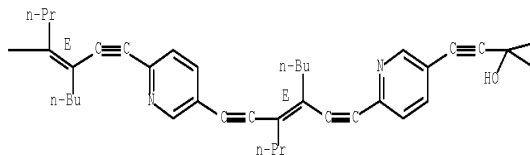
PAGE 1-B



PAGE 1-C



PAGE 1-B



OS.CITING REF COUNT: 20 THERE ARE 20 CAPLUS RECORDS THAT CITE THIS RECORD (20 CITINGS)  
 REFERENCE COUNT: 12 THERE ARE 12 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 11 OF 39 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 2004:328526 CAPLUS [Full-text](#)

DOCUMENT NUMBER: 141:54000

TITLE: Solid-phase synthesis of oligo(triacetylene)s and oligo(phenylenetriacetylene)s employing Sonogashira and Cadiot-Chodkiewicz-type cross-coupling reactions  
 AUTHOR(S): Utesch, Nils F.; Diederich, Francois; Boudon, Corinne; Gisselbrecht, Jean-Paul; Gross, Maurice



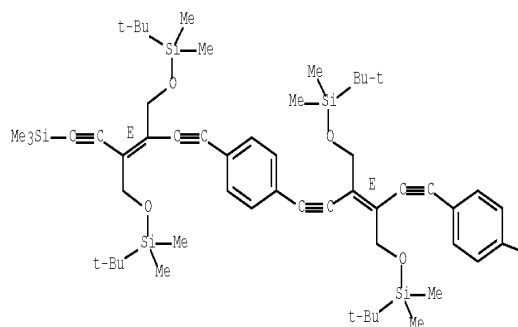
CORPORATE SOURCE: Laboratorium fuer Organische Chemie, ETH-Hoenggerberg,  
 HCl, Zurich, CH-8093, Switz.  
 SOURCE: Helvetica Chimica Acta (2004), 87(3), 698-718  
 CODEN: HCACAV; ISSN: 0018-019X  
 PUBLISHER: Verlag Helvetica Chimica Acta  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 OTHER SOURCE(S): CASREACT 141:54000

PAGE 1-A

AB The polymer-supported synthesis of poly(triacetylene)-derived monodisperse oligomers is described, using Pd0-catalyzed Sonogashira and Cadiot-Chodkiewicz-type cross-couplings as the key steps in the construction of the acetylenic scaffolds. Merrifield resin functionalized with a 1-(4-iodoaryl)triazene linker was chosen as the polymeric support. The linker selection was made based on the results of several model studies in the liquid phase. For the solid-support synthesis of p-I[C6H4C.tplbond.CC(CH2OSiMe2CMe3):C(CH2OSiMe2CMe3)C.tplbond.C]nSiMe3 [I, n = 2-4] a set of only three reactions was required: (i) Pd0-catalyzed Sonogashira cross-coupling, (ii) Me3Si-alkyne deprotection by protodesilylation, and (iii) cleavage of the linker with liberation of I. The longest-wavelength absorption maxima of I [n = 1-4] shift bathochromically with increasing oligomeric length, from  $\lambda_{\text{max}}$  337 nm (I, n = 1) to 384 nm (I, n = 4). Based on the electronic absorption data, the effective conjugation length (ECL) of the oligo(phenylene triacetylene)s is estimated to involve at least four monomer units and 40 C-atoms.  $\pi$ -Electron conjugation in these oligomers is less efficient than in Me3Si[C6H4C.tplbond.CC(CH2OSiMe2CMe3):C(CH2OSiMe2CMe3)C.tplbond.C]nSiMe3 (II) due to poor transmittance of  $\pi$ -electron delocalization by the Ph rings inserted into the oligomeric backbone. Similar conclusions were drawn from the electrochem. properties of the two oligomeric series as determined by cyclic (CV) and rotating-disk voltammetry. In sharp contrast to II, I are strongly fluorescent, with the highest quantum yield  $\Phi_F$  = 0.69 measured for I [n = 3]. Whereas the Sonogashira cross-coupling on solid support proceeded smoothly, optimal conditions for alkyne-alkyne cross-coupling reactions employing Pd0-catalyzed Cadiot-Chodkiewicz conditions still remain to be developed.

IT 554453-62-CP 554459-63-1P 554453-64-CP  
 RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)  
 (solid-phase synthesis of oligo(triacetylene)s and  
 oligo(phenylenetriacetylene)s by Sonogashira and Cadiot-Chodkiewicz  
 cross-coupling reactions)  
 RN 554459-62-0 CAPLUS  
 CN 4,9-Dioxa-3,10-disiladodec-6-ene, 6-[[4-[(3E)-3,4-bis[[[(1,1-dimethylethyl)dimethylsilyl]oxy]methyl]-6-(4-iodophenyl)-3-hexene-1,5-diynyl]phenyl]ethynyl]-2,2,3,3,10,10,11,11-octamethyl-7-[(trimethylsilyl)ethynyl]-, (6E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



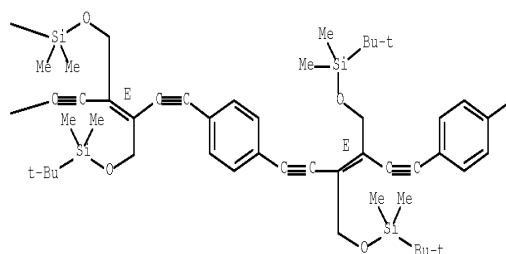
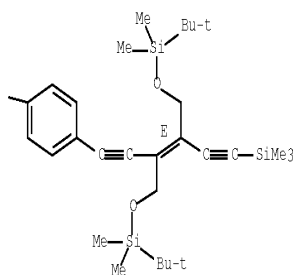
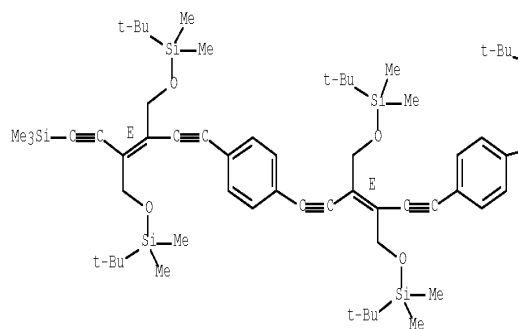
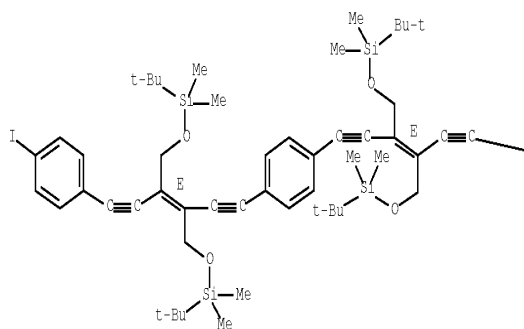
PAGE 1-B

I

RN 554459-63-1 CAPLUS  
 CN 4,9-Dioxa-3,10-disiladodec-6-ene, 6-[[4-[(3E)-6-[4-[(3E)-3,4-bis[[[(1,1-dimethylethyl)dimethylsilyl]oxy]methyl]-6-(4-iodophenyl)-3-hexene-1,5-diynyl]phenyl]-3,4-bis[[[(1,1-dimethylethyl)dimethylsilyl]oxy]methyl]-3-hexene-1,5-diynyl]phenyl]ethynyl]-2,2,3,3,10,10,11,11-octamethyl-7-[(trimethylsilyl)ethynyl]-, (6E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.





RN 554459-64-2 CAPLUS

CN 4,9-Dioxa-3,10-disiladodec-6-ene, 6-[[4-[(3E)-6-[4-[(3E)-3,4-bis[[[(1,1-dimethylethyl)dimethylsilyl]oxy]methyl]-6-(4-iodophenyl)-3-hexene-1,5-diynyl]phenyl]-3,4-bis[[[(1,1-dimethylethyl)dimethylsilyl]oxy]methyl]-3-hexene-1,5-diynyl]phenyl]ethynyl]-7-[[4-[(3E)-3,4-bis[[[(1,1-dimethylethyl)dimethylsilyl]oxy]methyl]-6-(trimethylsilyl)-3-hexene-1,5-diynyl]phenyl]ethynyl]-2,2,3,3,10,10,11,11-octamethyl-, (6E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

IT 704516-23-PP

RL: SPN (Synthetic preparation); PREP (Preparation)

(solid-phase synthesis of oligo(triacetylene)s and oligo(phenylenetriacetylene)s by Sonogashira and Cadiot-Chodkiewicz cross-coupling reactions)

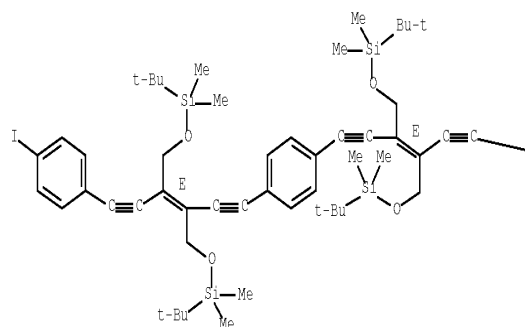
RN 704916-29-0 CAPLUS

CN 4,9-Dioxa-3,10-disiladodec-6-ene, 6,6'-(1,4-phenylenedi-2,1-ethynediyl)bis[7-[(4-iodophenyl)ethynyl]-2,2,3,3,10,10,11,11-octamethyl-, (6E,6'E)- (9CI) (CA INDEX NAME)

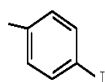
Double bond geometry as shown.



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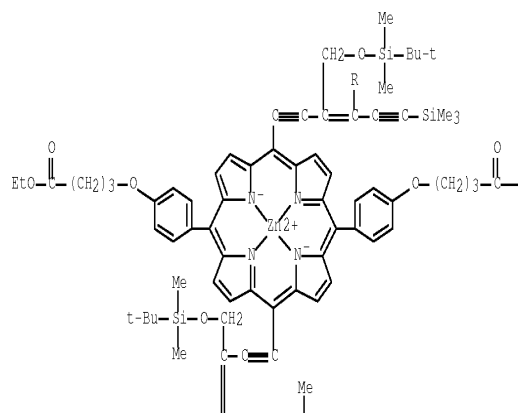


PAGE 1-B



dimethylethyl)dimethylsilyl]oxy)methyl]-6-(trimethylsilyl)-3-hexene-1,4-diyne]-21H,23H-porphine-5,15-diyl-  
 KN21,KN22,KN23,KN24]bis(4,1-phenyleneoxy)]bis[butanoato]](2-)]-, (SP-4-1)- (9CI) (CA INDEX NAME)

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OS.CITING REF COUNT: 6 THERE ARE 6 CAPLUS RECORDS THAT CITE THIS RECORD (6 CITINGS)  
 REFERENCE COUNT: 93 THERE ARE 93 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 12 OF 39 CAPLUS COPYRIGHT 2009 ACS on STN  
 ACCESSION NUMBER: 2003:1000504 CAPLUS [Full-text](#)  
 DOCUMENT NUMBER: 141:242819  
 TITLE: Product class 4: organometallic complexes of copper  
 AUTHOR(S): Heaney, H.; Christie, S.  
 CORPORATE SOURCE: Dept. of Chemistry, University of Loughborough, Loughborough, LE11 3TU, UK  
 SOURCE: Science of Synthesis (2004), 3, 305-662  
 CODEN: SSCYJ9  
 PUBLISHER: Georg Thieme Verlag  
 DOCUMENT TYPE: Journal; General Review  
 LANGUAGE: English

AB A review. The use of copper and related complexes in applications to organic synthesis is reviewed.

IT 219483-15-5P 375366-59-9P

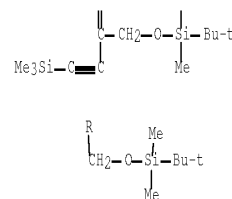
RL: SPN (Synthetic preparation); PREP (Preparation)  
 (applications of copper and organocopper complexes to organic synthesis)

RN 219483-15-5 CAPLUS

CN Zinc, [[diethyl 4,4'-[[[10,20-bis[(3E)-3,4-bis[[[(1,1-

—OEt

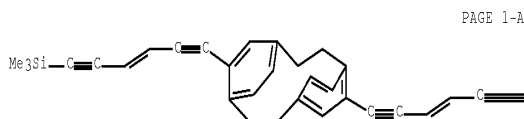
PAGE 2-A



RN 375366-59-9 CAPLUS  
 CN Tricyclo[8.2.2.24,7]hexadeca-4,6,10,12,13,15-hexaene,



5,11-bis[6-(trimethylsilyl)-3-hexene-1,5-diyn-1-yl]-, stereoisomer (CA INDEX NAME)



PAGE 1-B

OS.CITING REF COUNT: 5 THERE ARE 5 CAPLUS RECORDS THAT CITE THIS RECORD (5 CITINGS)  
 REFERENCE COUNT: 1706 THERE ARE 1706 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

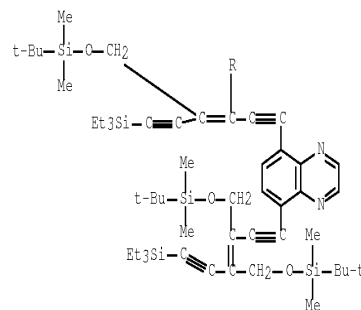
L8 ANSWER 13 OF 39 CAPLUS COPYRIGHT 2009 ACS on STN  
 ACCESSION NUMBER: 2003:592887 CAPLUS [Full-text](#)  
 DOCUMENT NUMBER: 140:20929  
 TITLE: Third-order nonlinear optical properties of in-backbone substituted oligo(triacetylene) chromophores  
 AUTHOR(S): Concilio, S.; Biaggio, I.; Gunter, P.; Piotto, S. P.; Edelman, M. J.; Raimundo, J.-M.; Diederich, F.  
 CORPORATE SOURCE: Swiss Federal Institute of Technology, Institute of Quantum Electronics, Nonlinear Optics Laboratory, ETH-Honggerberg, Zurich, CH-8093, Switz.  
 SOURCE: Journal of the Optical Society of America B: Optical Physics (2003), 20(8), 1656-1660  
 CODEN: JOBPDE; ISSN: 0740-3224  
 PUBLISHER: Optical Society of America  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English

AB A new approach to tuning the nonlinear optical properties of hybrid oligo(triacetylene) compds. was studied. The method is based on the insertion of a central heterospacer group between two (E)-hex-3-ene-1,5-diyne moieties. A significant increase in the 2nd hyperpolarizability  $\gamma$  is expected if the central spacer fragment is an extended conjugated chromophore. The authors present mols. with enhanced 2nd hyperpolarizability caused by the presence of highly conjugated spacer groups, which increase the overall  $\pi$ -electron delocalization. Some metal complexes obtained from the coordination of these hybrid oligomers to transition-metal centers also were studied and revealed substantial differences in the capacities of the metal centers to act as electronic bridges. Finally, theor. predictions of the relative differences in the 2nd hyperpolarizabilities of the new spacer compds. are in good agreement with the exptl. results.

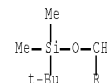
IT 628738-17-0 628738-18-1 628738-19-2

628738-20-5  
 RL: PRP (Properties)  
 (third-order nonlinear optical properties of in-backbone substituted oligo(triacetylene) chromophores)  
 RN 628738-17-0 CAPLUS  
 CN Quinoxaline, 5,8-bis[3,4-bis[[[(1,1-dimethylethyl)dimethylsilyl]oxy]methyl]-6-(triethylsilyl)-3-hexene-1,5-diynyl]- (9CI) (CA INDEX NAME)

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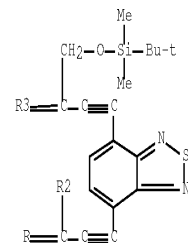


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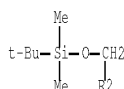
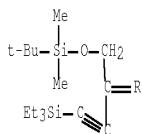
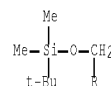


RN 628738-18-1 CAPLUS  
 CN 2,1,3-Benzothiadiazole, 4,7-bis[3,4-bis[[[(1,1-dimethylethyl)dimethylsilyl]oxy]methyl]-6-(triethylsilyl)-3-hexene-1,5-diyn-1-yl]- (CA INDEX NAME)

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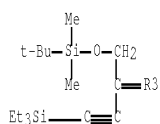
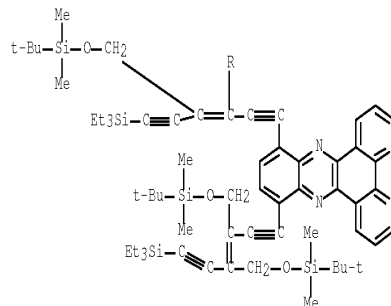






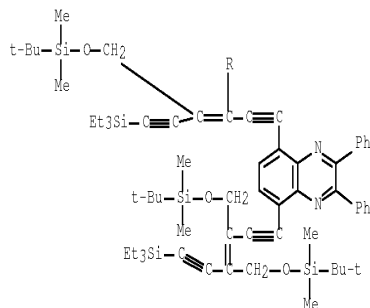
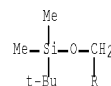
RN 628738-20-5 CAPLUS

CN Dipyrdo[3,2-a:2',3'-c]phenazine, 10,13-bis[3,4-bis[[[(1,1-dimethylethyl)dimethylsilyl]oxy]methyl]-6-(triethylsilyl)-3-hexene-1,5-diyne]- (9CI) (CA INDEX NAME)



RN 628738-19-2 CAPLUS

CN Quinoxaline, 5,8-bis[3,4-bis[[[(1,1-dimethylethyl)dimethylsilyl]oxy]methyl]-6-(triethylsilyl)-3-hexene-1,5-diyne]-2,3-diphenyl- (CA INDEX NAME)



OS.CITING REF COUNT: 4 THERE ARE 4 CAPLUS RECORDS THAT CITE THIS RECORD (4 CITINGS)

REFERENCE COUNT: 18 THERE ARE 18 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 14 OF 39 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 2003:491916 CAPLUS [Full-text](#)

DOCUMENT NUMBER: 139:395637

TITLE: Synthesis of differentially protected/functionalised acetylenic building blocks from p-benzoquinone and their use in the synthesis of new enediynes

AUTHOR(S): Sankararaman, Sethuraman; Srinivasan, Manivannan

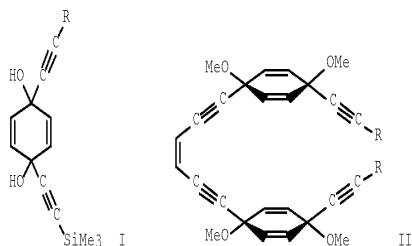
CORPORATE SOURCE: Department of Chemistry, Indian Institute of Technology Madras, Madras, 600 036, India

SOURCE: Organic & Biomolecular Chemistry (2003), 1(13), 2388-2392



PUBLISHER: CODEN: OBCRAK; ISSN: 1477-0520  
 DOCUMENT TYPE: Royal Society of Chemistry  
 LANGUAGE: Journal  
 OTHER SOURCE(S): English  
 CASREACT 139:395637  
 GI

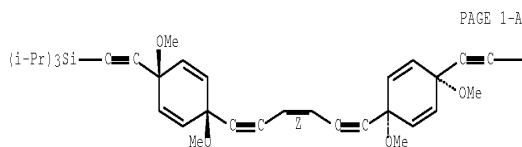
PAGE 1-B



AB Sequential addition of two different lithium acetylides to p-benzoquinone yielded diastereomeric mixts. of 1,4-diethynylcyclohexa-2,5-diene-1,4-diols I [R = (Me2CH)3Si, (EtO)2CH] with different protective/functional groups on the two ethynyl groups. Selective monodeprotection of the di-Me ethers of I to the corresponding terminal acetylenes followed by Pd(0)-mediated coupling with (Z)-1,2-dichloroethene yielded new enediynes II bearing cyclohexa-2,5-diene units.

IT 626235-20-9P  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
 (preparation of cyclohexadienyl enediynes via double addition of functionalized lithium acetylides to benzoquinone, selective monodeprotection and coupling with dichloroethene)  
 RN 626235-20-9 CAPLUS  
 CN Silane, [(3Z)-3-hexene-1,5-diyne-1,6-diylbis[(cis-1,4-dimethoxy-2,5-cyclohexadiene-1,4-diyl)-2,1-ethynediyl]]bis[tris(1-methylethyl)- (9CI) (CA INDEX NAME)]

Relative stereochemistry.  
 Double bond geometry as shown.

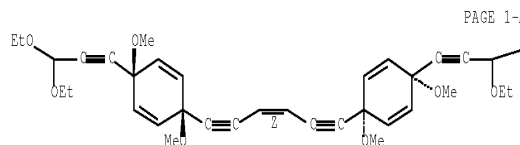


PAGE 1-A



IT 626235-21-0P 626235-22-1P  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (preparation of cyclohexadienyl enediynes via double addition of functionalized lithium acetylides to benzoquinone, selective monodeprotection and coupling with dichloroethene)  
 RN 626235-21-0 CAPLUS  
 CN 1,4-Cyclohexadiene, 3,3'-(3Z)-3-hexene-1,5-diyne-1,6-diylbis[6-(3,3-diethoxy-1-propynyl)-3,6-dimethoxy-, (cis,cis)- (9CI) (CA INDEX NAME)]

Relative stereochemistry.  
 Double bond geometry as shown.



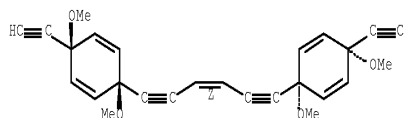
PAGE 1-A



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RN 626235-22-1 CAPLUS  
 CN 1,4-Cyclohexadiene, 3,3'-(3Z)-3-hexene-1,5-diyne-1,6-diylbis[6-ethynyl-3,6-dimethoxy-, (cis,cis)- (9CI) (CA INDEX NAME)]

Relative stereochemistry.  
 Double bond geometry as shown.



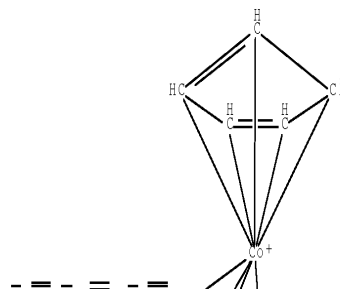
OS.CITING REF COUNT: 6 THERE ARE 6 CAPLUS RECORDS THAT CITE THIS RECORD (6 CITINGS)  
 REFERENCE COUNT: 17 THERE ARE 17 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 15 OF 39 CAPLUS COPYRIGHT 2009 ACS on STN



ACCESSION NUMBER: 2003:345601 CAPLUS Full-text  
 DOCUMENT NUMBER: 139:149735  
 TITLE: Butterfly topologies: new expanded carbon-rich organometallic scaffolds  
 AUTHOR(S): Laskoski, Matthew; Roidl, Gaby; Ricks, Holly L.; Morton, Jason G. M.; Smith, Mark D.; Bunz, Uwe H. F.  
 CORPORATE SOURCE: USC NanoCenter, Department of Chemistry and Biochemistry, The University of South Carolina, Columbia, SC, 29208, USA  
 SOURCE: Journal of Organometallic Chemistry (2003), 673(1-2), 13-24  
 CODEN: JORCAI; ISSN: 0022-328X  
 PUBLISHER: Elsevier Science B.V.  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 OTHER SOURCE(S): CASREACT 139:149735  
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PAGE 1-A



\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

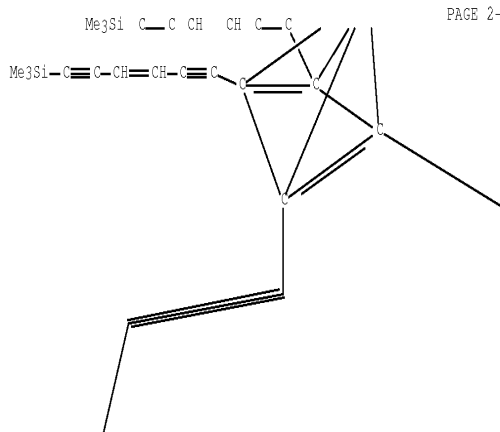
AB Starting from either (tetraethynylcyclobutadiene)cyclopentadienylcobalt or [1,2-diethynyl-3,4-(2-dioxanyl)cyclobutadiene]cyclopentadienylcobalt a sequence of copper and Pd-catalyzed couplings of the Eglinton and Heck-Cassar-Sonogashira-Hagihara type furnished five bow-tie shaped doubly annulated dehydroannulenes, the largest of which featured a (formal) 7,8:13,14:25,26:31,32-tetra(4'-alkyl-1',2'-benzo)tricyclo[18,16,02,19]hexatricosa-3,5,9,11,15,17,21,23,27,29,33,35-dodecayne-1,7,13,19,25,31-hexaene hydrocarbon ligand with a cyclopentadienylcobalt-stabilized cyclobutadiene complex as its central unit (I) (R = i-Pr, n-Bu). Single crystal X-ray structures of two of the smaller butterflies (II) and (III) are reported and their surprising solid-state packing is discussed herein. The solid state structure of III was also examined via PM3 calcs.

IT 349453-20-9P  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation, crystal structure, and PM3 calcn. of butterfly dehydro[14]annulenes and dehydro[18]annulenes containing a cyclobutadiene(cyclopentadienyl)cobalt unit)

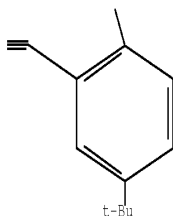
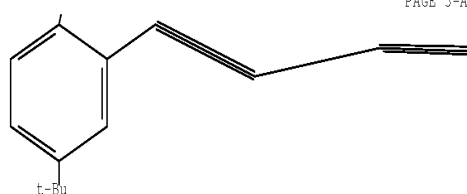
RN 349453-20-9 CAPLUS

CN Cobalt, (η<sup>5</sup>-2,4-cyclopentadien-1-yl)[[(1,2,2a,18a-η)-3,4,9,10,11,12,17,18-octadehydro-7,14-bis(1,1-dimethylethyl)dibenzo[a,i]cyclobuta[e]cyclotetradecene-1,2-diyl]di-(3Z)-3-hexene-1,5-diyne-6,1-diyl]bis(trimethylsilane)]- (9CI) (CA INDEX NAME)



PAGE 2-A





TITLE: Acetylenic scaffolding on solid support:  
Poly(triacetylene)-derived oligomers by Sonogashira and Cadiot-Chodkiewicz-type cross-coupling reactions

AUTHOR(S): Utesch, Nils F.; Diederich, Francois

CORPORATE SOURCE: Laboratorium fur Organische Chemie, ETH-Honggerberg, HCI, Zurich, CH-8093, Switz.

SOURCE: Organic & Biomolecular Chemistry (2003), 1(2), 237-239  
CODEN: OBCRAK; ISSN: 1477-0520

PUBLISHER: Royal Society of Chemistry

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 139:85055

AB Synthesis of poly(triacetylene)-derived oligomers by Pd(0)-catalyzed Sonogashira and Cadiot-Chodkiewicz-type cross-coupling reactions on solid support is reported. Oligo(phenylene triacetylene)s, e.g., I[4-C6H4C.tplbond.CCR:CR:CR.tplbond.C]nSiMe3 (R = CH2OSiButMe2, n = 1, 2, 3, 4) members of a new class of linearly  $\pi$ -conjugated oligomers with all-C backbones, feature very high fluorescence intensities.

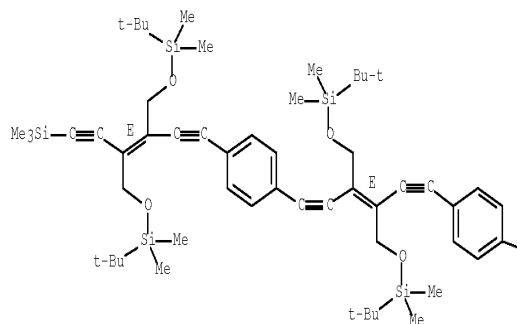
IT 554459-62-0P 554459-63-1P 554459-64-2P

RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation) (electronic absorption and emission, UV/VIS spectra; poly(triacetylene)-derived oligomers are prepared by Sonogashira and Cadiot-Chodkiewicz-type Pd-catalyzed cross-coupling reactions)

RN 554459-62-0 CAPLUS

CN 4,9-Dioxa-3,10-disiladodec-6-ene, 6-[[4-[(3E)-3,4-bis[[[(1,1-dimethylethyl)dimethylsilyl]oxy]methyl]-6-(4-iodophenyl)-3-hexene-1,5-diynyl]phenyl]ethynyl]-2,2,3,3,10,10,11,11-octamethyl-7-[(trimethylsilyl)ethynyl]-, (6E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



OS.CITING REF COUNT: 11 THERE ARE 11 CAPLUS RECORDS THAT CITE THIS RECORD (11 CITINGS)

REFERENCE COUNT: 81 THERE ARE 81 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 16 OF 39 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 2003:234291 CAPLUS [Full-text](#)

DOCUMENT NUMBER: 139:85055

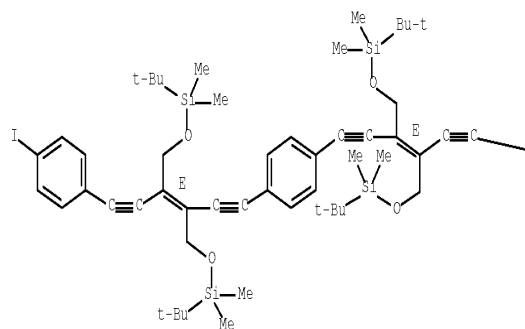


-I

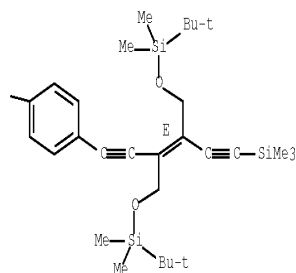
RN 554459-63-1 CAPLUS

CN 4,9-Dioxa-3,10-disiladodec-6-ene, 6-[[4-[(3E)-6-[4-[(3E)-3,4-bis[[[(1,1-dimethylethyl)dimethylsilyl]oxy]methyl]-6-(4-iodophenyl)-3-hexene-1,5-diynyl]phenyl]-3,4-bis[[[(1,1-dimethylethyl)dimethylsilyl]oxy]methyl]-3-hexene-1,5-diynyl]phenyl]ethynyl]-2,2,3,3,10,10,11,11-octamethyl-7-[(trimethylsilyl)ethynyl]-, (6E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



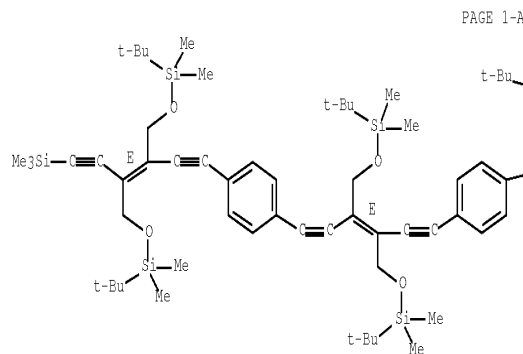
PAGE 1-A



RN 554459-64-2 CAPLUS

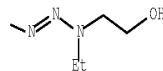
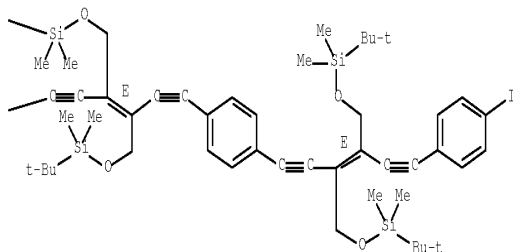
CN 4,9-Dioxa-3,10-disiladodec-6-ene, 6-[[4-[(3E)-6-[4-[(3E)-3,4-bis[[[(1,1-dimethylethyl)dimethylsilyl]oxy]methyl]-6-(4-iodophenyl)-3-hexene-1,5-diynyl]phenyl]-3,4-bis[[[(1,1-dimethylethyl)dimethylsilyl]oxy]methyl]-3-hexene-1,5-diynyl]phenyl]ethynyl]-7-[[4-[(3E)-3,4-bis[[[(1,1-dimethylethyl)dimethylsilyl]oxy]methyl]-6-(trimethylsilyl)-3-hexene-1,5-diynyl]phenyl]ethynyl]-2,2,3,3,10,10,11,11-octamethyl-, (6E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



PAGE 1-A





IT 554459-71-1DP, Merrifield resin-supported  
 554459-73-3GP, Merrifield resin-supported 554459-73-3GP  
 , Merrifield resin-supported  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT  
 (Reactant or reagent)

(preparation and Sonogashira and Cadiot-Chodkiewicz-type Pd-catalyzed  
 cross-coupling reactions of supported poly(triacetylene)-derived  
 oligomers)

RN 554459-71-1 CAPLUS

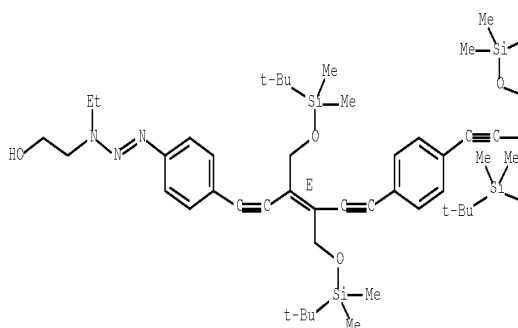
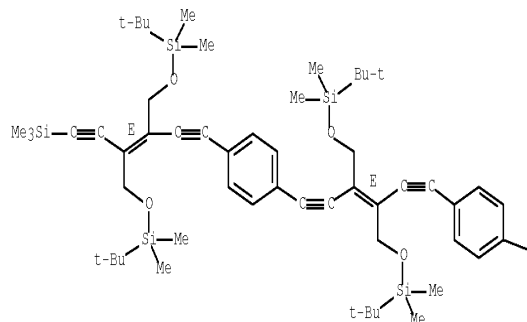
CN Ethanol, 2-[3-[4-[(3E)-6-[4-[(3E)-3,4-bis[[[(1,1-  
 dimethylethyl)dimethylsilyl]oxy]methyl]-6-(trimethylsilyl)-3-hexene-1,5-  
 diyn-1-yl]phenyl]-3,4-bis[[[(1,1-dimethylethyl)dimethylsilyl]oxy]methyl]-3-  
 hexene-1,5-diyn-1-yl]phenyl]-1-ethyl-2-triazene-1-yl]- (CA INDEX NAME)

Double bond geometry as described by E or Z.

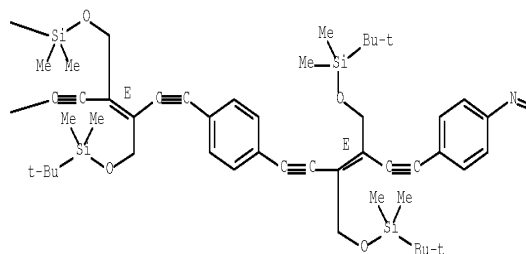
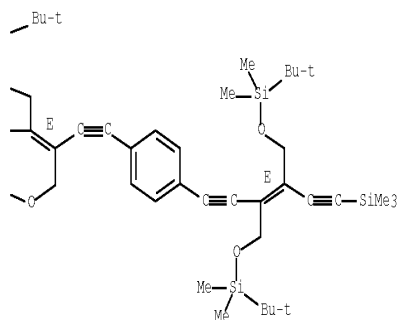
RN 554459-72-2 CAPLUS

CN Ethanol, 2-[3-[4-[(3E)-6-[4-[(3E)-3,4-bis[[[(1,1-  
 dimethylethyl)dimethylsilyl]oxy]methyl]-6-(trimethylsilyl)-3-hexene-1,5-  
 diyn-1-yl]phenyl]-3,4-bis[[[(1,1-dimethylethyl)dimethylsilyl]oxy]methyl]-3-  
 hexene-1,5-diyn-1-yl]phenyl]-3,4-bis[[[(1,1-  
 dimethylethyl)dimethylsilyl]oxy]methyl]-3-hexene-1,5-diyn-1-yl]phenyl]-1-  
 ethyl-2-triazene-1-yl]- (CA INDEX NAME)

Double bond geometry as described by E or Z.



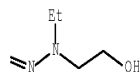




RN 554459-73-3 CAPLUS

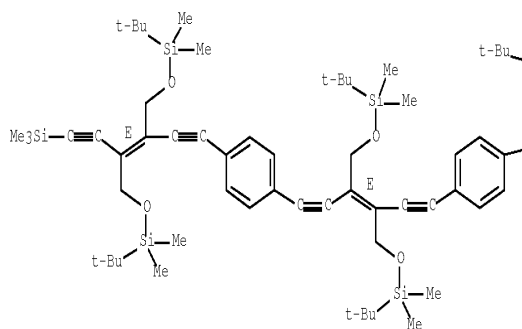
CN Ethanol, 2-[3-[4-[(3E)-6-[4-[(3E)-6-[4-[(3E)-3,4-bis[[[(1,1-dimethylethyl)dimethylsilyl]oxy]methyl]-6-(trimethylsilyl)-3-hexene-1,5-diyn-1-yl]phenyl]-3,4-bis[[[(1,1-dimethylethyl)dimethylsilyl]oxy]methyl]-3-hexene-1,5-diyn-1-yl]phenyl]-3,4-bis[[[(1,1-dimethylethyl)dimethylsilyl]oxy]methyl]-3-hexene-1,5-diyn-1-yl]phenyl]-3,4-bis[[[(1,1-dimethylethyl)dimethylsilyl]oxy]methyl]-3-hexene-1,5-diyn-1-yl]phenyl]-1-ethyl-2-triazen-1-yl]- (CA INDEX NAME)

PAGE 1-C



Double bond geometry as described by E or Z.

PAGE 1-A



OS.CITING REF COUNT: 18 THERE ARE 18 CAPLUS RECORDS THAT CITE THIS RECORD (18 CITINGS)  
 REFERENCE COUNT: 38 THERE ARE 38 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 17 OF 39 CAPLUS COPYRIGHT 2009 ACS ON STN  
 ACCESSION NUMBER: 2002:874017 CAPLUS [Full-text](#)  
 DOCUMENT NUMBER: 138:72938  
 TITLE: Diatropicity of 3,4,7,8,9,10,13,14-Octadehydro[14]annulenes: A Combined Experimental and Theoretical Investigation  
 AUTHOR(S): Boydston, Andrew J.; Haley, Michael M.; Williams, Richard Vaughan; Armantrout, John R.  
 CORPORATE SOURCE: Department of Chemistry, University of Oregon, Eugene, OR, 97403-1253, USA  
 SOURCE: Journal of Organic Chemistry (2002), 67(25), 8812-8819  
 CODEN: JOCEAH; ISSN: 0022-3263  
 PUBLISHER: American Chemical Society  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 OTHER SOURCE(S): CASREACT 138:72938  
 AB The synthesis and study of a series of octadehydro[14]annulenes is described. The aromaticity of these annulenes was investigated through examination of exptl. data from arene-fused systems as well as calculated nucleus-independent chemical shifts (NICS) and bond lengths. Benzene ring fusion to the parent system results in a stepwise loss in aromaticity as the number of fused rings is increased from one to two to three. This decrease in annulenic ring current is manifested in the alkene proton chemical shifts (0-2 benzenes) as well as the NICS (0-3 benzenes). Comparison of isomeric thiophene-fused



annulenes shows further evidence of ring current competition as these allow for observation of intermittent degrees of delocalization throughout the annulenic core. A consistent relationship between the magnitude of the NICS values and the degree of benzannulation is also observed

IT 482294-13-3P

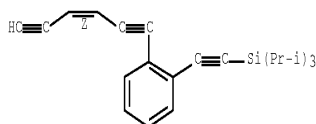
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(cross-coupling; a combined exptl. and theor. investigation of diatropicity of 3,4,7,8,9,10,13,14-octadehydro[14]annulenes)

RN 482294-19-9 CAPLUS

CN Benzene, 1-(3Z)-3-hexene-1,5-diyn-1-yl-2-[2-(tris(1-methylethyl)silyl)ethynyl]- (CA INDEX NAME)

Double bond geometry as shown.



IT 482294-17-7P 482294-20-2P 482294-21-3P

482294-22-4P

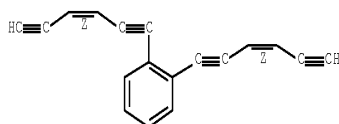
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(cyclization; a combined exptl. and theor. investigation of diatropicity of 3,4,7,8,9,10,13,14-octadehydro[14]annulenes)

RN 482294-17-7 CAPLUS

CN Benzene, 1,2-di(3Z)-3-hexene-1,5-diyn-1-yl- (CA INDEX NAME)

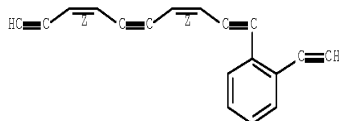
Double bond geometry as shown.



RN 482294-20-2 CAPLUS

CN Benzene, 1-(3Z,7Z)-3,7-decadiene-1,5,9-triyn-1-yl-2-ethynyl- (CA INDEX NAME)

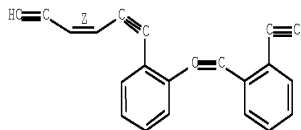
Double bond geometry as shown.



RN 482294-21-3 CAPLUS

CN Benzene, 1-ethynyl-2-[[2-(3Z)-3-hexene-1,5-diynylphenyl]ethynyl]- (9CI) (CA INDEX NAME)

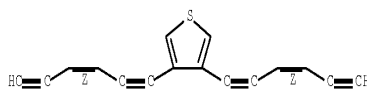
Double bond geometry as shown.



RN 482294-22-4 CAPLUS

CN Thiophene, 3,4-di(3Z)-3-hexene-1,5-diyn-1-yl- (CA INDEX NAME)

Double bond geometry as shown.



IT 482294-15-5P

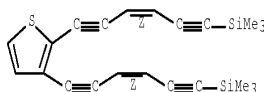
RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(deprotection/cyclization; a combined exptl. and theor. investigation of diatropicity of 3,4,7,8,9,10,13,14-octadehydro[14]annulenes)

RN 482294-15-5 CAPLUS

CN Thiophene, 2,3-bis[(3Z)-6-(trimethylsilyl)-3-hexene-1,5-diyn-1-yl]- (CA INDEX NAME)

Double bond geometry as shown.



IT 381173-15-5P 381173-20-2P 482294-13-3P

482294-14-4P

RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

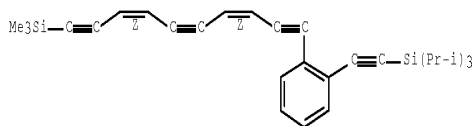
(deprotection; a combined exptl. and theor. investigation of diatropicity of 3,4,7,8,9,10,13,14-octadehydro[14]annulenes)

RN 381173-15-5 CAPLUS

CN Benzene, 1-[(3Z,7Z)-10-(trimethylsilyl)-3,7-decadiene-1,5,9-triyn-1-yl]-2-[2-(tris(1-methylethyl)silyl)ethynyl]- (CA INDEX NAME)

Double bond geometry as shown.



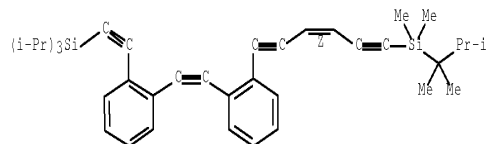


PAGE 1-B

—Si(Pr-i)<sub>3</sub>

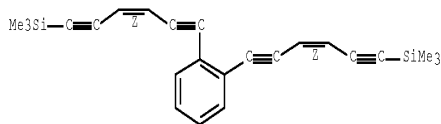
RN 381173-20-2 CAPLUS  
 CN Silane, [1,2-bis[(3Z)-6-[dimethyl(1,1,2-trimethylpropyl)silyl]-3-hexene-1,5-diynyl]phenyl]ethynyl]phenyl]ethynyl]tris(1-methylethyl)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



RN 482294-13-3 CAPLUS  
 CN Silane, [1,2-phenylenedi-(3Z)-3-hexene-1,5-diyne-6,1-diyl]bis(trimethyl- (9CI) (CA INDEX NAME)

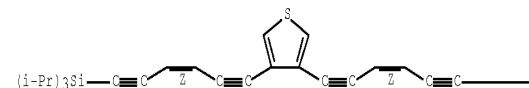
Double bond geometry as shown.



RN 482294-14-4 CAPLUS  
 CN Thiophene, 3,4-bis[(3Z)-6-[tris(1-methylethyl)silyl]-3-hexene-1,5-diyn-1-yl]- (CA INDEX NAME)

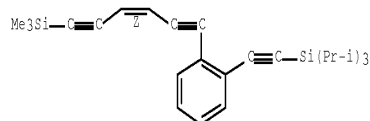
Double bond geometry as shown.

PAGE 1-A



IT 381173-13-3P  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
 (deprotection; a combined exptl. and theor. investigation of diatropicity of 3,4,7,8,9,10,13,14-octadehydro[14]annulenes)  
 RN 381173-13-3 CAPLUS  
 CN Benzene, 1-[(3Z)-6-(trimethylsilyl)-3-hexene-1,5-diyn-1-yl]-2-[2-[tris(1-methylethyl)silyl]ethynyl]- (CA INDEX NAME)

Double bond geometry as shown.



OS.CITING REF COUNT: 31 THERE ARE 31 CAPLUS RECORDS THAT CITE THIS RECORD (33 CITINGS)  
 REFERENCE COUNT: 44 THERE ARE 44 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 18 OF 39 CAPLUS COPYRIGHT 2009 ACS on STN  
 ACCESSION NUMBER: 2002:874016 CAPLUS [Full-text](#)  
 DOCUMENT NUMBER: 138:72902  
 TITLE: Dimethyldihydropyrene-Dehydrobenzoannulene Hybrids: Studies in Aromaticity and Photoisomerization  
 AUTHOR(S): Kimball, David B.; Haley, Michael M.; Mitchell, Reginald H.; Ward, Timothy R.; Bandyopadhyay, Subhajit; Williams, Richard Vaughan; Armantrout, John R.  
 CORPORATE SOURCE: Department of Chemistry and the Materials Science Institute, University of Oregon, Eugene, OR, 97403-1253, USA  
 SOURCE: Journal of Organic Chemistry (2002), 67(25), 8798-8811  
 CODEN: JOCEAH; ISSN: 0022-3263  
 PUBLISHER: American Chemical Society  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 OTHER SOURCE(S): CASREACT 138:72902  
 AB The synthesis and study of dehydrobenzoannulene (DBA)-dimethyldihydropyrene (DDP) hybrids as models for the investigation of aromaticity in weakly diatropic systems is reported. Three new monofused DBA-DDP hybrids have been synthesized, and their NMR spectra are discussed with regard to quantifying the aromaticity remaining in multibenzene-fused DBAs. Nucleus-independent chemical shifts, determined at a series of locations for each compound, bond lengths, and <sup>1</sup>H and <sup>13</sup>C NMR chemical shifts were calculated and used to probe



the aromaticity of these hybrids. Systems where more than one annulene/DBA is fused to the DDP core have also been obtained, and their potential use in photoinduced isomerization applications is discussed.

IT 481713-23-9E

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

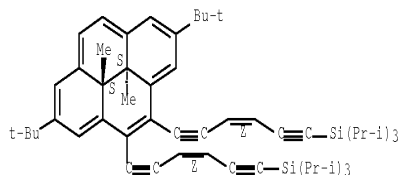
(desilylation/cyclization; studies in aromaticity and photoisomerization of dimethyldihydropyrene-dehydrobenzoannulene hybrids)

RN 481713-23-9 CAPLUS

CN Pyrene, 2,7-bis(1,1-dimethylethyl)-10b,10c-dihydro-10b,10c-dimethyl-4,5-bis[(3Z)-6-[tris(1-methylethyl)silyl]-3-hexene-1,5-diyn-1-yl]-, (10bR,10cR)-rel- (CA INDEX NAME)

Relative stereochemistry.

Double bond geometry as shown.



OS.CITING REF COUNT: 21 THERE ARE 21 CAPLUS RECORDS THAT CITE THIS RECORD (21 CITINGS)

REFERENCE COUNT: 78 THERE ARE 78 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 19 OF 39 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 2002:719354 CAPLUS [Full-text](#)

DOCUMENT NUMBER: 138:25161

TITLE: Third-order nonlinear optical properties of in-backbone substituted conjugated polymers

AUTHOR(S): Gubler, U.; Concilio, S.; Bosshard, Ch.; Biaggio, I.; Gunter, P.; Martin, R. E.; Edelman, M. J.; Wytko, J. A.; Diederich, F.

CORPORATE SOURCE: Institute of Quantum Electronics, ETH-Honggerberg, Zurich, CH-8093, Switz.

SOURCE: Applied Physics Letters (2002), 81(13), 2322-2324 CODEN: APPLAB; ISSN: 0003-6951

PUBLISHER: American Institute of Physics

DOCUMENT TYPE: Journal

LANGUAGE: English

AB An alternative approach for tuning of the third-order nonlinear optical properties of organic mols. is based on insertion a functional group into the path of the  $\pi$ -electron conjugation instead of at chain ends. This scheme enhances the second-order hyperpolarizability for short mols., but in two instances where such mols. were polymerized into longer mols. the overall hyperpolarizability was lower. The study is based on tert-butyltrimethylsiloxy-vinyl-poly(triacetylene) as the basic linear conjugated polymer, with spacer of anthracene, benzene, naphthalene, thiophene, tetramethylbenzene, furan tetrafluorobenzene, pyridine, biphenyl, pyrazine, and bis(triethylphosphine-Pt).

IT 249616-79-3 249616-82-8,

2,6-Bis[(E)-3,4-bis[[tert-butyl]dimethylsilyloxy]methyl]-6-(trimethylsilyl)-hex-3-ene-1,5-diynyl]naphthalene 249616-83-3, 9,10-Bis[(E)-3,4-bis[[tert-butyl]dimethylsilyloxy]methyl]-6-(trimethylsilyl)-hex-3-ene-1,5-diynyl]anthracene 249616-84-0

249616-87-3, 1,4-Bis[(E)-3,4-bis[[tert-butyl]dimethylsilyloxy]methyl]-6-(trimethylsilyl)-hex-3-ene-1,5-diynyl]-2,3,5,6-tetramethylbenzene 249616-88-4 249616-89-5

, 2,5-Bis[(E)-3,4-bis[[tert-butyl]dimethylsilyloxy]methyl]-6-(trimethylsilyl)-hex-3-ene-1,5-diynyl]pyrazine 249616-90-8

249616-91-3, 2,5-Bis[(E)-3,4-bis[[tert-butyl]dimethylsilyloxy]methyl]-6-(trimethylsilyl)-hex-3-ene-1,5-diynyl]furan

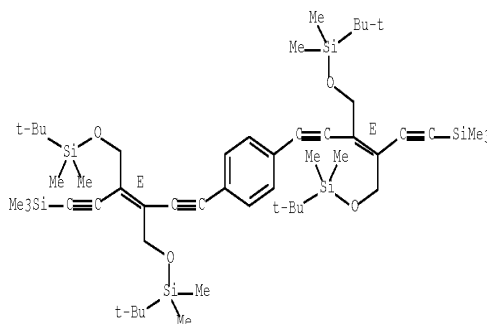
RL: PRP (Properties)

(role of in-backbone spacer on third-order nonlinear optical properties of polyacetylene conjugated polymers)

RN 249616-79-3 CAPLUS

CN 4,9-Dioxa-3,10-disiladodec-6-ene, 6,6'-(1,4-phenylenedi-2,1-ethynediyl)bis[2,2,3,3,10,10,11,11-octamethyl-7-[(trimethylsilyl)ethynyl]-, (6E,6'E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



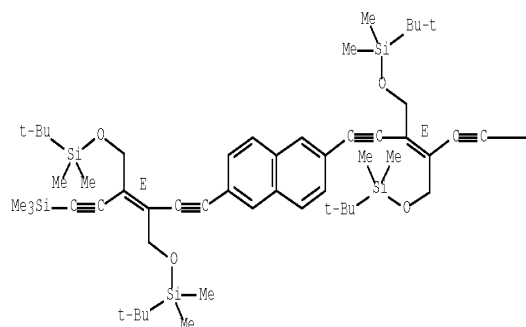
RN 249616-82-8 CAPLUS

CN 4,9-Dioxa-3,10-disiladodec-6-ene, 6,6'-(2,6-naphthalenediyl)-2,1-ethynediyl]bis[2,2,3,3,10,10,11,11-octamethyl-7-[(trimethylsilyl)ethynyl]-, (6E,6'E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



PAGE 1-A



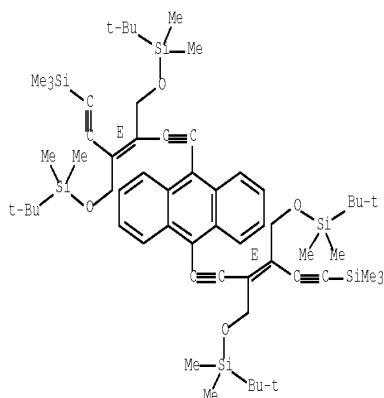
PAGE 1-B

—SiMe<sub>3</sub>

RN 249616-83-9 CAPLUS

CN 4,9-Dioxo-3,10-disiladodec-6-ene, 6,6'-[(9,10-anthracenediyl)di-2,1-ethynediyl]bis[2,2,3,3,10,10,11,11-octamethyl-7-[(trimethylsilyl)ethynyl]-, (6E,6'E)- (9CI) (CA INDEX NAME)

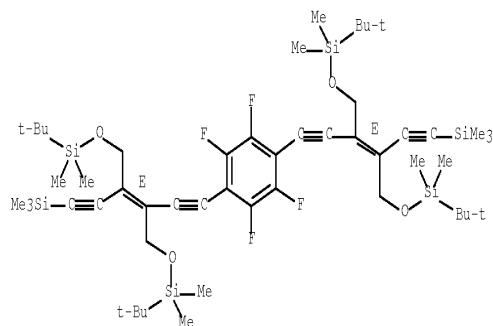
Double bond geometry as shown.



RN 249616-84-0 CAPLUS

CN 4,9-Dioxo-3,10-disiladodec-6-ene, 6,6'-[(2,3,5,6-tetrafluoro-1,4-phenylene)di-2,1-ethynediyl]bis[2,2,3,3,10,10,11,11-octamethyl-7-[(trimethylsilyl)ethynyl]-, (6E,6'E)- (9CI) (CA INDEX NAME)

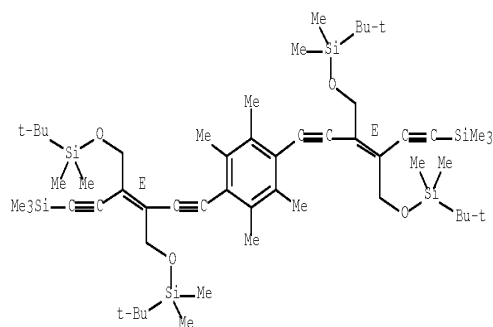
Double bond geometry as shown.



RN 249616-87-3 CAPLUS

CN 4,9-Dioxo-3,10-disiladodec-6-ene, 6,6'-[(2,3,5,6-tetramethyl-1,4-phenylene)di-2,1-ethynediyl]bis[2,2,3,3,10,10,11,11-octamethyl-7-[(trimethylsilyl)ethynyl]-, (6E,6'E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

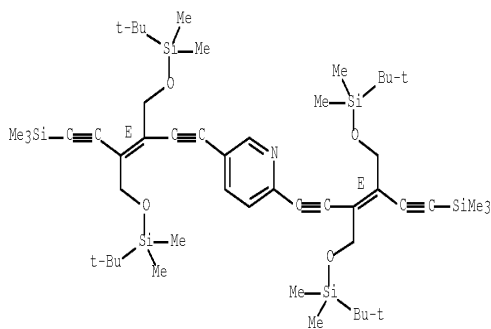


RN 249616-88-4 CAPLUS

CN Pyridine, 2,5-bis[(3E)-3,4-bis[[[(1,1-dimethylethyl)dimethylsilyl]oxy]methyl]-6-(trimethylsilyl)-3-hexene-1,5-diyn-1-yl]- (CA INDEX NAME)

Double bond geometry as shown.

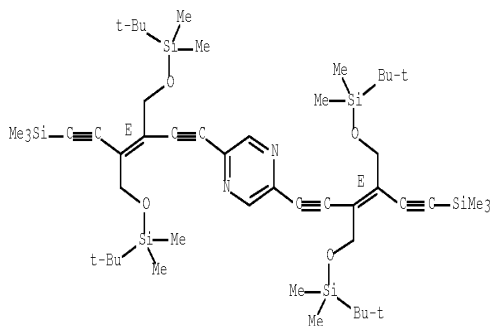




RN 249616-89-5 CAPLUS

CN Pyrazine, 2,5-bis[(3E)-3,4-bis[[[(1,1-dimethylethyl)dimethylsilyl]oxy]methyl]-6-(trimethylsilyl)-3-hexene-1,5-diyn-1-yl]- (CA INDEX NAME)

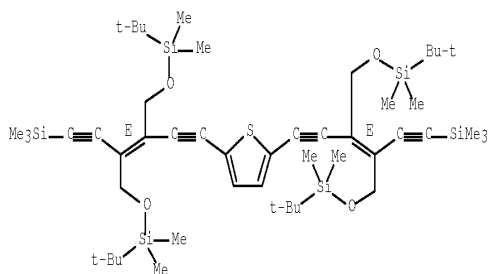
Double bond geometry as shown.



RN 249616-90-8 CAPLUS

CN 4,9-Dioxo-3,10-disiladodec-6-ene, 6,6'-(2,5-thiophenediyl)-2,1-ethynediylbis[2,2,3,3,10,10,11,11-octamethyl-7-[(trimethylsilyl)ethynyl]-, (6E,6'E)- (9CI) (CA INDEX NAME)

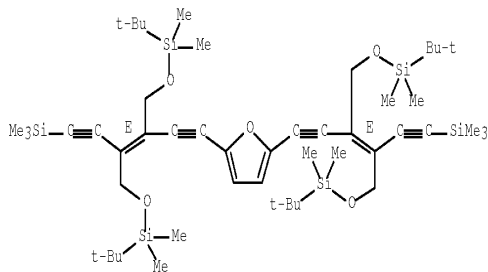
Double bond geometry as shown.



RN 249616-91-9 CAPLUS

CN 4,9-Dioxo-3,10-disiladodec-6-ene, 6,6'-(2,5-furandiyl)-2,1-ethynediylbis[2,2,3,3,10,10,11,11-octamethyl-7-[(trimethylsilyl)ethynyl]-, (6E,6'E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



OS.CITING REF COUNT: 15 THERE ARE 15 CAPLUS RECORDS THAT CITE THIS RECORD (15 CITINGS)

REFERENCE COUNT: 11 THERE ARE 11 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 20 OF 39 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 2002:700080 CAPLUS [Full-text](#)

DOCUMENT NUMBER: 138:247934

TITLE: Cytotoxicities and topoisomerase I inhibitory activities of 2-[2-(2-alkynylphenyl)ethynyl]benzonitriles, 1-aryldec-3-ene-1,5-diynes, and related bis(enediynyl)arene compounds

AUTHOR(S): Lin, Chi-Fong; Lu, Wen-Der; Hsieh, Pei-Chen; Kuo, Yao-Haur; Chiu, Huey-Fen; Wang, Chyi-Jia; Wu, Ming-Jung

CORPORATE SOURCE: School of Chemistry, Kaohsiung Medical University, Kaohsiung, Taiwan

SOURCE: Helvetica Chimica Acta (2002), 85(8), 2564-2575

CODEN: HCACAV; ISSN: 0018-019X

PUBLISHER: Verlag Helvetica Chimica Acta



OTHER SOURCE(S): CASREACT 138:247934

AB The activities of a series of acyclic enediynes, 2-(6-substituted hex-3-ene-1,5-diynyl)benzonitriles (1-5) and their derivs. 7-23 were evaluated against several solid tumor cell lines and topoisomerase I. Comps. 1-5 show selective cytotoxicity with Hepa cells, and 2-[6-phenylhex-3-ene-1,5-diynyl]benzonitrile (5) reveals the most-potent activity. Analogs 8-10 and 13-22 also have the same effect with DLD cells; 1-[(Z)-dec-3-ene-1,5-diynyl]-4-nitrobenzene (21) shows the highest activity among them. Moreover, 1-[(Z)-dec-3-ene-1,5-diynyl]-2-(trifluoromethyl)benzene (20) exhibits the strongest inhibitory activity with the Hela cell line. Derivs. 9, 10, 18, and 23 display inhibitory activities with topoisomerase I at 87  $\mu$ M. The cell-cycle anal. of compound 5, which induces a significant blockage in S phase, indicates that these novel enediynes probably undergo other biol. pathways leading to the cytotoxicity, except the inhibitory activity toward topoisomerase I.

IT 457914-65-70

RL: PAC (Pharmacological activity); PRP (Properties); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

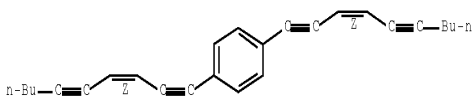
(cytotoxicity and topoisomerase I inhibitory activity of

2-[2-(2-alkynylphenyl)ethynyl]benzonitriles,  
1-aryldec-3-ene-1,5-diynes, and related bis(enediynyl)arene compds.)

RN 457914-65-7 CAPLUS

CN Benzene, 1,4-di(3Z)-3-decene-1,5-diyn-1-yl- (CA INDEX NAME)

Double bond geometry as shown.



OS.CITING REF COUNT: 3 THERE ARE 3 CAPLUS RECORDS THAT CITE THIS RECORD  
(3 CITINGS)

REFERENCE COUNT: 7 THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS  
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 21 OF 39 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 2002:628032 CAPLUS Full-text

DOCUMENT NUMBER: 138:4578

TITLE: Dramatically enhanced fluorescence of heteroaromatic  
chromophores upon insertion as spacers into  
oligo(triacetylene)s

AUTHOR(S): Edelmann, Michael J.; Raimundo, Jean-Manuel; Utesch, Nils E.; Diederich, Francois

CORPORATE SOURCE: Lab. Organische Chemie, ETH-Hoenggerberg, HCI, Zurich,  
CH-8093, Switz.

SOURCE: Helvetica Chimica Acta (2002), 85(7), 2195-2213

CODEN: HCACAV; ISSN: 0018-019X

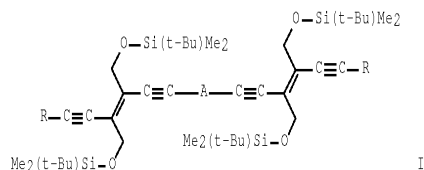
PUBLISHER: Verlag Helvetica Chimica Acta

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 138:4578

GT



AB In continuation of a previous study on the modulation of  $\pi$ -electron conjugation of oligo(triacetylene)s by insertion of central hetero-spacer fragments between two (E)-hex-3-ene-1,5-diyne ((E)-1,2-diethynylethene, DEE) moieties, trimeric hybrid oligomers (I; A = spacer, R = SiEt<sub>3</sub>, SiMe<sub>3</sub>) were prepared. Spacers used were both electron-deficient (quinoxaline-based heterocycles, pyridazine) and electron-rich (2,2'-bithiophene, 9,9-dioctyl-9H-fluorene) chromophores. With a dipyrrophenazine spacer, transition metal complexes were synthesized as potential precursors for nanoscale scaffolding based on both covalent acetylenic coupling and supramol. assembly. The UV/visible spectra revealed that the majority of spacers provided heterotrimers featuring extended  $\pi$ -electron delocalization. The new hybrid chromophores show a dramatically enhanced fluorescence compared with the DEE dimer and homo-trimer. This increase in emission intensity appears as a general feature of these systems: even if the spacer mol. is nonfluorescent, the corresponding hetero-trimer may show a strong emission. The redox properties of the new hybrid chromophores were determined by cyclic voltammetry (CV) and rotating disk voltammetry (RDV). In each case, the first 1-electron reduction step in the hetero-trimers appeared anodically shifted compared with DEE dimer and homo-trimer. With larger spacer chromophore extending into two dimensions, the anodic shift (by 240-490 mV) seems to originate from inductive effects of the two strongly electron-accepting DEE substituents rather than from extended  $\pi$ -electron conjugation along the oligomeric backbone, as had previously been observed for DEE substituted porphyrins.

IT	477293-98-4P	477295-99-5P	477294-00-1P
	477294-01-2P	477294-02-3P	477294-03-5P
	477294-06-7P	477294-08-9P	477294-09-0P
	477294-11-4P		

RL: CPS (Chemical process); PEP (Physical, engineering or chemical process); PRP (Properties); SPN (Synthetic preparation); PREP (Preparation); PROC (Process)

```
(preparation, electrochem. properties and dramatically enhanced fluorescence
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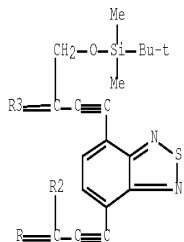
of compds. consisting of heteroarom. chromophores inserted as spacers into oligo(triacetylene)s)

RN 477293-98-4 CAPLUS

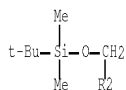
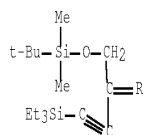
CN 2,1,3-Benzothiadiazole, 4,7-bis[[3E]-3,4-bis[[[(1,1-dimethylethyl)dimethylsilyl]oxy]methyl]-6-(triethylsilyl)-3-hexene-1,5-divin-1-yl]- (CA INDEX NAME)



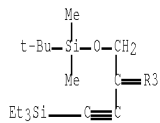
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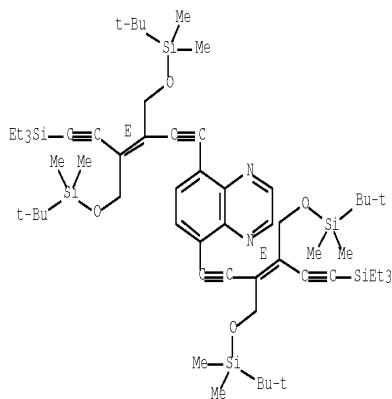
PAGE 3-A



RN 477293-99-5 CAPLUS

CN Quinoxaline, 5,8-bis[(3E)-3,4-bis[[(1,1-dimethylethyl)dimethylsilyl]oxy]methyl]-6-(triethylsilyl)-3-hexene-1,5-diynyl]- (9CI) (CA INDEX NAME)

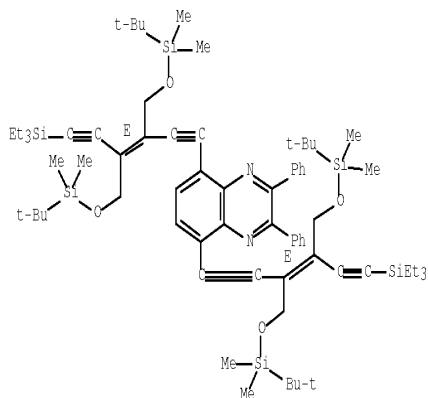
Double bond geometry as shown.



RN 477294-00-1 CAPLUS

CN Quinoxaline, 5,8-bis[(3E)-3,4-bis[[(1,1-dimethylethyl)dimethylsilyl]oxy]methyl]-6-(triethylsilyl)-3-hexene-1,5-diynyl]-2,3-diphenyl- (CA INDEX NAME)

Double bond geometry as shown.



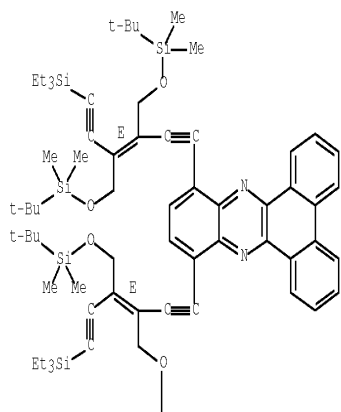
RN 477294-01-2 CAPLUS

CN Dibenzo[a,c]phenazine, 10,13-bis[(3E)-3,4-bis[[(1,1-dimethylethyl)dimethylsilyl]oxy]methyl]-6-(triethylsilyl)-3-hexene-1,5-diynyl]- (CA INDEX NAME)

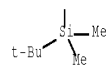
Double bond geometry as shown.



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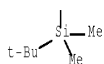


RN 477294-04-5 CAPLUS  
 CN Zinc(2+), bis[10,13-bis[(3E)-3,4-bis[[(1,1-dimethylethyl)dimethylsilyl]oxy]methyl]-6-(triethylsilyl)-3-hexene-1,5-diynyl]dipyrido[3,2-a:2',3'-c]phenazine-KN4,KN5]-, (T-4)-, salt with trifluoromethanesulfonic acid (1:2) (9CI) (CA INDEX NAME)

CM 1

CRN 477294-03-4  
 CMF C140 H212 N8 O8 Si12 Zn  
 CCI CCS

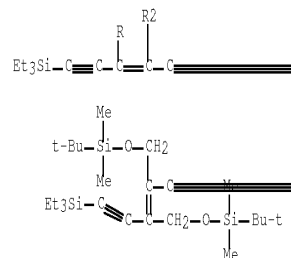
PAGE 2-A



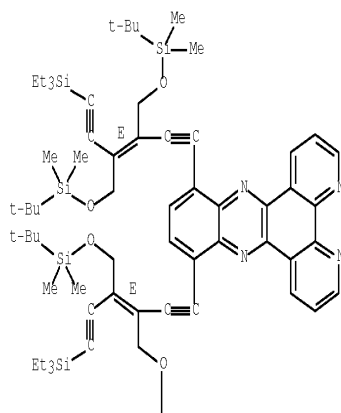
PAGE 1-A

RN 477294-02-3 CAPLUS  
 CN Dipyrdo[3,2-a:2',3'-c]phenazine, 10,13-bis[(3E)-3,4-bis[[(1,1-dimethylethyl)dimethylsilyl]oxy]methyl]-6-(triethylsilyl)-3-hexene-1,5-diynyl]- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

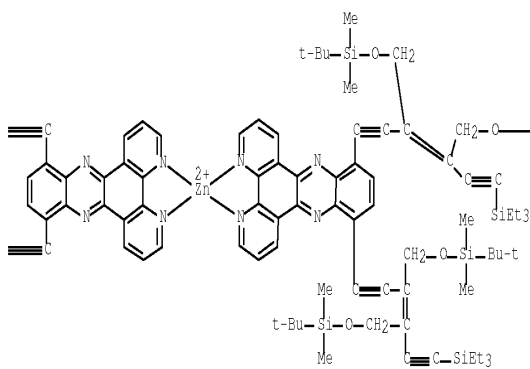


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RN 477294-06-7 CAPLUS

CN Nickel (2+), bis[10,13-bis[(3E)-3,4-bis[[[(1,1-dimethylethyl)dimethylsilyl]oxy]methyl]-6-(triethylsilyl)-3-hexene-1,5-diynyl]dipyrido[3,2-a:2',3'-c]phenazine-κN4,κN5]-, (T-4)-, diperchlorate (9CI) (CA INDEX NAME)

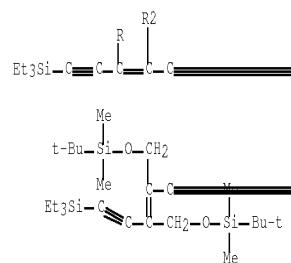
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CRN 477294-05-6

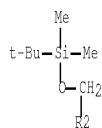
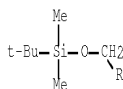
CMF C140 H212 N8 Ni O8 Si12

CCI CCS

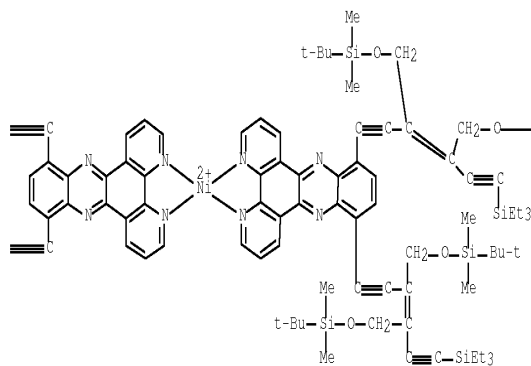
PAGE 1-A



PAGE 2-A



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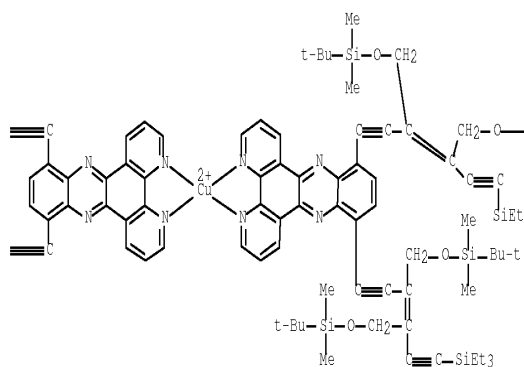
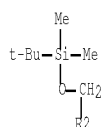
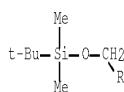
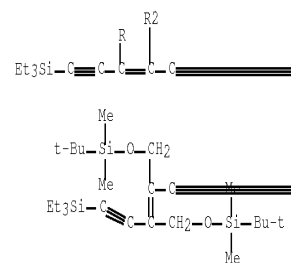


CM 2

CRN 37181-39-8

CMF C F3 O3 S





CM 2

CRN 14797-73-0

CMF Cl O4



RN 477294-08-9 CAPLUS

CN Copper (2+), bis[10,13-bis[(3E)-3,4-bis[[[(1,1-dimethylethyl)dimethylsilyl]oxy]methyl]-6-(triethylsilyl)-3-hexene-1,5-diynyl]dipyrido[3,2-a:2',3'-c]phenazine-KN4,KN5]-, (T-4)-, bis[hexafluorophosphate(1-)] (9CI) (CA INDEX NAME)

CM 1

CRN 477294-07-8

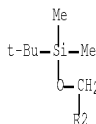
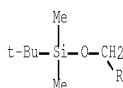
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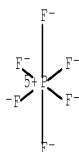


PAGE 2-A



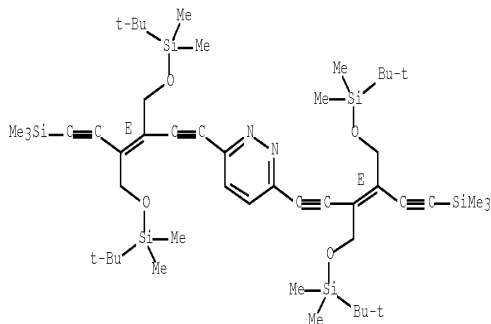
CM 2

CRN 16919-18-9  
CMF F6 P  
CCI CCS



RN 477294-09-0 CAPLUS  
CN Pyridazine, 3,6-bis[(3E)-3,4-bis[[[(1,1-dimethylethyl)dimethylsilyl]oxy]methyl]-6-(trimethylsilyl)-3-hexene-1,5-diyn-1-yl]- (CA INDEX NAME)

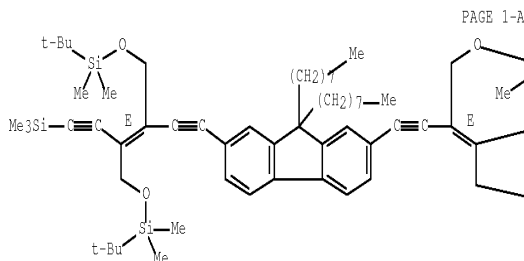
Double bond geometry as shown.



RN 477294-11-4 CAPLUS

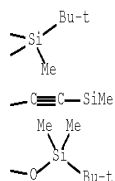
CN 4,9-Dioxo-3,10-disiladodec-6-ene, 6,6'-[(9,9-dioctyl-9H-fluorene-2,7-diyl)di-2,1-ethynediyl]bis[2,2,3,3,10,10,11,11-octamethyl-7-[(trimethylsilyl)ethynyl]-, (6E,6'E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



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PAGE 1-B



OS.CITING REF COUNT: 42 THERE ARE 42 CAPLUS RECORDS THAT CITE THIS RECORD (44 CITINGS)  
REFERENCE COUNT: 44 THERE ARE 44 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 22 OF 39 CAPLUS COPYRIGHT 2009 ACS on STN  
ACCESSION NUMBER: 2002:539072 CAPLUS [Full-text](#)  
DOCUMENT NUMBER: 137:232177  
TITLE: Anionic Cycloaromatization of 1-Aryl-3-hexen-1,5-diynes Initiated by Methoxide Addition: Synthesis of Phenanthridinones, Benzo[c]phenanthridinones, and Biaryls  
AUTHOR(S): Wu, Ming-Jung; Lin, Chi-Fong; Lu, Wen-Der  
CORPORATE SOURCE: School of Chemistry, Kaohsiung Medical University, Kaohsiung, Taiwan  
SOURCE: Journal of Organic Chemistry (2002), 67(17), 5907-5912  
CODEN: JOCEAH; ISSN: 0022-3263  
PUBLISHER: American Chemical Society  
DOCUMENT TYPE: Journal  
LANGUAGE: English  
OTHER SOURCE(S): CASREACT 137:232177  
AB Treatment of 2-((Z)-6-substituted-3-hexene-1,5-diynyl)benzonitriles with sodium methoxide in refluxing methanol in the presence of a polar aprotic solvent, such as DMSO, HMPA, THF, or 18-crown-6, gave phenanthridinones in 21-



77% yields. In these cases, addition of 10% DMSO into the reaction mixture gave the highest yield. On the other hand, methanolysis of 2-(2-(2-alkynylphenyl)ethynyl)benzonitriles under the same reaction conditions gave benzo[c]phenanthridinones in 31-57% yields. Methanolysis of (Z)-1-aryl-3-hexene-1,5-diynes in the presence of 2 equiv of tetrabutylammonium iodide gave biaryls in 14-64% yields. It is found that the reactions with aryl groups bearing electron-withdrawing groups proceeded at greater rates and gave better yields.

IT 457914-65-7P

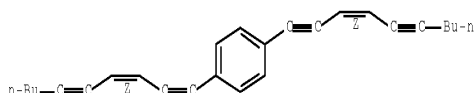
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(anionic cycloaromatization of 1-aryl-3-hexene-1,5-diynes initiated by addition of methanol)

RN 457914-65-7 CAPLUS

CN Benzene, 1,4-di(3Z)-3-decene-1,5-diyn-1-yl- (CA INDEX NAME)

Double bond geometry as shown.



OS.CITING REF COUNT: 13 THERE ARE 13 CAPLUS RECORDS THAT CITE THIS RECORD (13 CITINGS)

REFERENCE COUNT: 15 THERE ARE 15 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 23 OF 39 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 2002:471478 CAPLUS [Full-text](#)

DOCUMENT NUMBER: 137:310580

TITLE: Evaluation of ring-strain effects in cycloalkene-fused octadehydro[14]annulenes

AUTHOR(S): Boydston, A. J.; Laskoski, Matthew; Bunz, Uwe H. F.; Haley, Michael M.

CORPORATE SOURCE: Department of Chemistry, University of Oregon, Eugene, OR, 97403-1253, USA

SOURCE: Synlett (2002), (6), 981-983

CODEN: SYNLES; ISSN: 0936-5214

PUBLISHER: Georg Thieme Verlag

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 137:310580

AB The possibility of ring strain as the cause of bond localization in metalloarene-fused octadehydro[14]annulenes is addressed. It was found that strain-induced bond localization is not observable in the mildly aromatic annulenes previously used to compare the degree of delocalization in CpCo(cyclobutadiene) relative to ferrocene and benzene.

IT 472956-26-6P 472956-28-8P

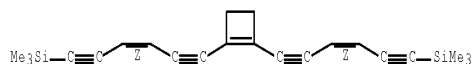
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(deprotection/cyclization; evaluation of ring-strain effects in cycloalkene-fused octadehydro[14]annulenes)

RN 472956-26-6 CAPLUS

CN Cyclobutene, 1,2-bis[(3Z)-6-(trimethylsilyl)-3-hexene-1,5-diyn-1-yl]- (CA INDEX NAME)

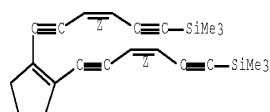
Double bond geometry as shown.



RN 472956-28-8 CAPLUS

CN Cyclopentene, 1,2-bis[(3Z)-6-(trimethylsilyl)-3-hexene-1,5-diyn-1-yl]- (CA INDEX NAME)

Double bond geometry as shown.



OS.CITING REF COUNT: 6 THERE ARE 6 CAPLUS RECORDS THAT CITE THIS RECORD (6 CITINGS)

REFERENCE COUNT: 13 THERE ARE 13 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 24 OF 39 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 2001:731976 CAPLUS [Full-text](#)

DOCUMENT NUMBER: 136:53492

TITLE: Diatropicity of Dehydrobenzo[14]annulenes: Comparative Analysis of the Bond-Fixing Ability of Benzene on the Parent 3,4,7,8,9,10,13,14-Octadehydro[14]annulene

AUTHOR(S): Boydston, A. J.; Haley, Michael M.

CORPORATE SOURCE: Department of Chemistry, University of Oregon, Eugene, OR, 97403-1253, USA

SOURCE: Organic Letters (2001), 3(22), 3599-3601

CODEN: ORLEF7; ISSN: 1523-7060

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 136:53492

AB We report the synthesis of 3,4,7,8,9,10,13,14-octadehydro[14]annulene and detail a comparative aromaticity study with its benzannulated derivs. (e.g., benzo[e]-3,4,7,8,9,10,13,14-octadehydro[14]annulene and dibenzo[a,e]-3,4,7,8,9,10,13,14-octadehydro[14]annulene).

IT 381173-13-3P 381173-15-6P 381173-20-2P

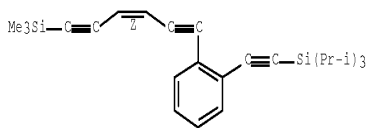
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation) (intermediate; diatropicity of dehydrobenzoannulenes)

RN 381173-13-3 CAPLUS

CN Benzene, 1-[(3Z)-6-(trimethylsilyl)-3-hexene-1,5-diyn-1-yl]-2-[2-(1-methylethyl)silyl]ethynyl]- (CA INDEX NAME)

Double bond geometry as shown.

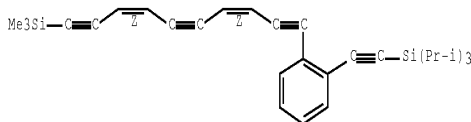




CODEN: EJOCFK; ISSN: 1434-193X  
 PUBLISHER: Wiley-VCH Verlag GmbH  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 OTHER SOURCE(S): CASREACT 136:69640  
 GI

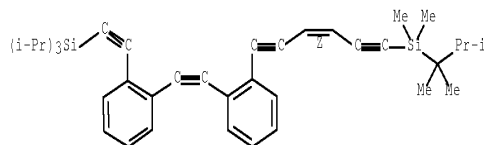
RN 381173-15-5 CAPLUS  
 CN Benzene, 1-[(3Z,7Z)-10-(trimethylsilyl)-3,7-decadiene-1,5,9-triyn-1-yl]-2-[2-[tris(1-methylethyl)silyl]ethynyl]- (CA INDEX NAME)

Double bond geometry as shown.



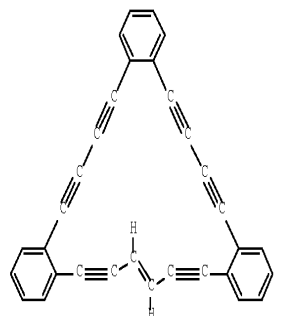
RN 381173-20-2 CAPLUS  
 CN Silane, [[2-[[2-[(3Z)-6-[dimethyl(1,1,2-trimethylpropyl)silyl]-3-hexene-1,5-diynyl]phenyl]ethynyl]phenyl]ethynyl]tris(1-methylethyl)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



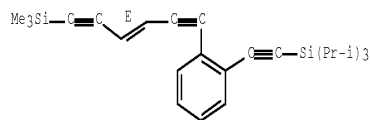
OS.CITING REF COUNT: 19 THERE ARE 19 CAPLUS RECORDS THAT CITE THIS RECORD (19 CITINGS)  
 REFERENCE COUNT: 20 THERE ARE 20 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 25 OF 39 CAPLUS COPYRIGHT 2009 ACS on STN  
 ACCESSION NUMBER: 2001:714296 CAPLUS [Full-text](#)  
 DOCUMENT NUMBER: 136:69640  
 TITLE: Synthesis and spectroscopic studies of expanded planar dehydrotribenzo[n]annulenes containing one or two isolated alkene units  
 AUTHOR(S): Wan, W. Brad; Chiechi, Ryan C.; Weakley, Timothy J. R.; Haley, Michael M.  
 CORPORATE SOURCE: Department of Chemistry and the Materials Science Institute, University of Oregon, Eugene, OR, 97403-1253, USA  
 SOURCE: European Journal of Organic Chemistry (2001), (18), 3485-3490



AB Dehydrobenzoannulene derivs. containing isolated alkene linkages, e.g., I, were synthesized by combining an in situ Pd/Cu-mediated cross-coupling with an intramol. cyclization strategy. 1H NMR studies of these macrocycles and comparison with related systems verify that highly alkynylated dehydrobenzoannulenes possess weak induced ring currents, indicative of aromatic (4n+2  $\pi$  systems) and antiarom. (4n  $\pi$  systems) behavior, in spite of their large size and extensive benzannulation.  
 IT 214628-16-7P 214623-17-8P 214628-18-9P  
 383494-33-4P  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
 (preparation and spectroscopic studies of expanded planar dehydrotribenzo[n]annulenes containing one or two isolated alkene units)  
 RN 214628-16-7 CAPLUS  
 CN Benzene, 1-[(3E)-6-(trimethylsilyl)-3-hexene-1,5-diyn-1-yl]-2-[2-[tris(1-methylethyl)silyl]ethynyl]- (CA INDEX NAME)

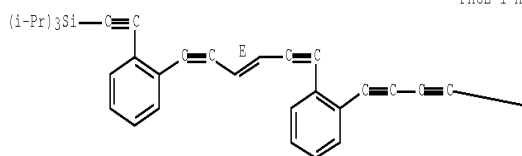
Double bond geometry as shown.



RN 214628-17-8 CAPLUS  
 CN Silane, tris(1-methylethyl)[[2-[(3E)-6-[2-[4-[2-[[tris(1-methylethyl)silyl]ethynyl]phenyl]-1,3-butadiynyl]phenyl]-3-hexene-1,5-diynyl]phenyl]ethynyl]- (9CI) (CA INDEX NAME)

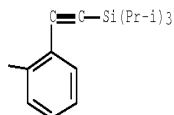


Double bond geometry as shown.



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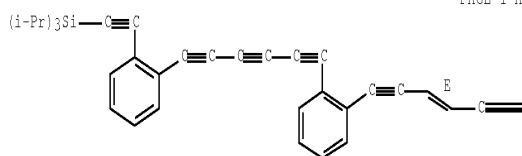
PAGE 1-B



RN 214628-18-9 CAPLUS

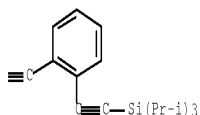
CN Silane, tris(1-methylethyl)[[2-[6-[2-[(3E)-6-[2-[[tris(1-methylethyl)silyl]ethynyl]phenyl]-3-hexene-1,5-diynyl]phenyl]-1,3,5-hexatriynyl]phenyl]ethynyl]- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



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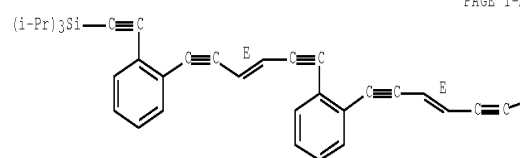
PAGE 1-B



RN 383404-38-4 CAPLUS

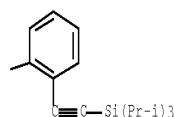
CN Silane, [1,2-phenylenebis[(3E)-3-hexene-1,5-diyne-6,1-diyl-2,1-phenylene-2,1-ethynediyl]]bis[tris(1-methylethyl)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



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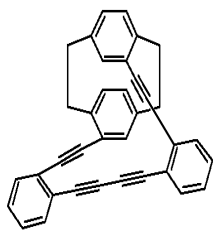
PAGE 1-B



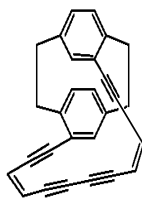
OS.CITING REF COUNT: 10 THERE ARE 10 CAPLUS RECORDS THAT CITE THIS RECORD (10 CITINGS)  
REFERENCE COUNT: 33 THERE ARE 33 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 26 OF 39 CAPLUS COPYRIGHT 2009 ACS on STN  
ACCESSION NUMBER: 2001:664308 CAPLUS [Full-text](#)  
DOCUMENT NUMBER: 136:5789  
TITLE: [2.2]Paracyclophane/dehydrobenzoannulene hybrids: Transannular delocalization in open-circuited conjugated macrocycles  
AUTHOR(S): Boydston, A. J.; Bondarenko, Lidija; Dix, Ina; Weakley, Timothy J. R.; Hopf, Henning; Haley, Michael M.  
CORPORATE SOURCE: Institut fur Organische Chemie, Technische Universitat Braunschweig, Braunschweig, 38106, Germany  
SOURCE: Angewandte Chemie, International Edition (2001), 40(16), 2986-2989  
CODEN: ACIEF5; ISSN: 1433-7851  
PUBLISHER: Wiley-VCH Verlag GmbH  
DOCUMENT TYPE: Journal  
LANGUAGE: English  
OTHER SOURCE(S): CASREACT 136:5789  
GI





I



II

AB Formylation and following alkynylation of dibromoparacyclophane gave dialkynylparacyclophane as key for the synthesis of [2.2]paracyclophane/dehydrobenzoannulene hybrids I and II. I and II were assembled by Pd-catalyzed cross-coupling of iodoarene and chloroalkene with dialkynylparacyclophane and subsequent cyclization. The study of the transannular delocalization in open-circuited conjugated macrocycles using optical properties and the elucidation of solid-stated structure of II by x-ray crystallog. [monoclinic, P2<sub>1</sub>/n, a 9.505(2), b 15.077(2), c 13.687(2) Å, β 98.608(8), V 1939.3(6) Å<sup>3</sup>, Z 4] are reported.

IT 375366-59-96

RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(preparation and transannular delocalization of open-circuited conjugated paracyclophane/dehydrobenzoannulene macrocycles)

RN 375366-59-9 CAPLUS

CN Tricyclo[8.2.2.2<sup>4</sup>,7]hexadeca-4,6,10,12,13,15-hexaene, 5,11-bis[6-(trimethylsilyl)-3-hexene-1,5-diyn-1-yl]-, stereoisomer (CA INDEX NAME)

ACCESSION NUMBER: 2001:481503 CAPLUS [Full-text](#)  
DOCUMENT NUMBER: 135:211133  
TITLE: Organometallic Dehydro[14]annulenes Containing Vollhardt's Cyclobutadiene: Are CpCo-Complexed Cyclobutadienes More Aromatic than Benzene?  
AUTHOR(S): Laskoski, Matthew; Smith, Mark D.; Morton, Jason G. M.; Bunz, Uwe H. F.  
CORPORATE SOURCE: Department of Chemistry and Biochemistry, The University of South Carolina, Columbia, SC, 29208, USA  
SOURCE: Journal of Organic Chemistry (2001), 66(15), 5174-5181  
CODEN: JOCEAH; ISSN: 0022-3263  
PUBLISHER: American Chemical Society  
DOCUMENT TYPE: Journal  
LANGUAGE: English  
OTHER SOURCE(S): CASREACT 135:211133

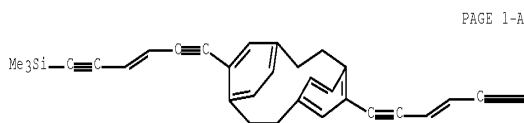
AB Pd-catalyzed coupling of [1,2-diethynyl-3,4-bis(trimethylsilyl)cyclobutadiene](cyclopentadienyl)cobalt to a series of 1-iodo-2-(trimethylsilylethynyl)benzenes and 1-chloro-4-trimethylsilylbut-1-ene-3-yne is followed by desilylation with potassium carbonate. Cu(OAc)<sub>2</sub>-promoted oxidative ring closure leads to dehydro[14]annulenes and dehydro[14]benzoannulenes fused to a cyclobutadiene(cyclopentadienylcobalt) complex. Five of these fused dehydroannulenes were structurally characterized. <sup>1</sup>H NMR spectroscopy of the organometallic dehydro[14]annulenes incorporating the (bistrimethylsilyl)cyclobutadiene(cyclopentadienylcobalt) unit suggested that the aromaticity of the fused cyclobutadiene complex might be stronger than that of benzene according to the ring-current criterion.

IT 350586-85-5 350586-94-6

RL: PRP (Properties)  
(NMR and aromaticity of)

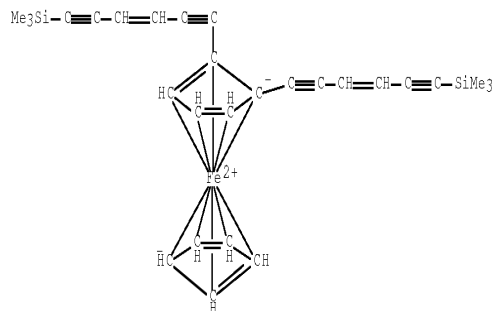
RN 350586-85-5 CAPLUS

CN Ferrocene, 1,2-bis[(3Z)-6-(trimethylsilyl)-3-hexene-1,5-diynyl]- (9CI) (CA INDEX NAME)



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RN 350586-94-6 CAPLUS

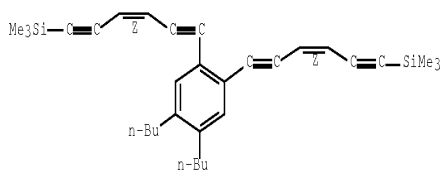
CN Silane, [(4,5-dibutyl-1,2-phenylene)di-(3Z)-3-hexene-1,5-diyn-6,1-diyl]bis(trimethyl- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

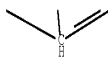
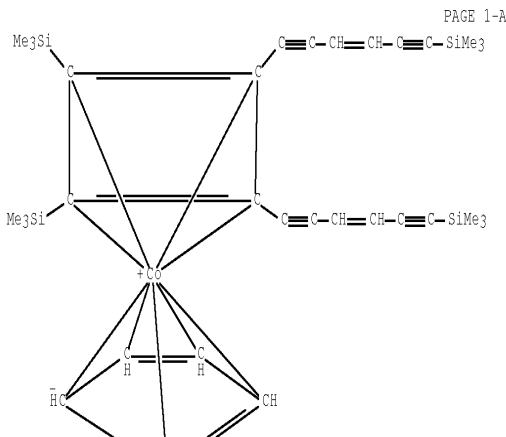
OS.CITING REF COUNT: 20 THERE ARE 20 CAPLUS RECORDS THAT CITE THIS RECORD (20 CITINGS)  
REFERENCE COUNT: 33 THERE ARE 33 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 27 OF 39 CAPLUS COPYRIGHT 2009 ACS on STN



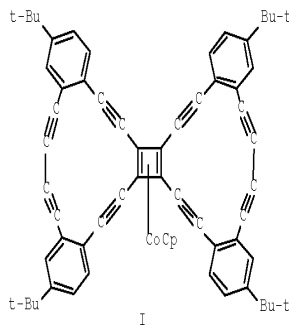


IT 358365-18-1P  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT  
 (Reactant or reagent)  
 (preparation, desilylation, and sequential copper-catalyzed oxidative ring  
 closure of)  
 RN 358365-18-1 CAPLUS  
 CN Cobalt, [[[1,2,3,4- $\eta$ ]-3,4-bis(trimethylsilyl)-1,3-cyclobutadiene-1,2-  
 diyl]di-(3Z)-3-hexene-1,5-diyne-6,1-diyl]bis(trimethylsilane)]( $\eta^5$ -2,4-  
 cyclopentadien-1-yl)- (9CI) (CA INDEX NAME)



PAGE 2-A

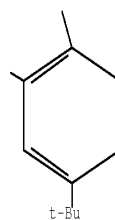
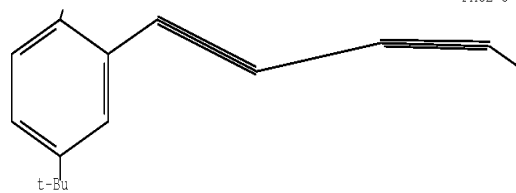
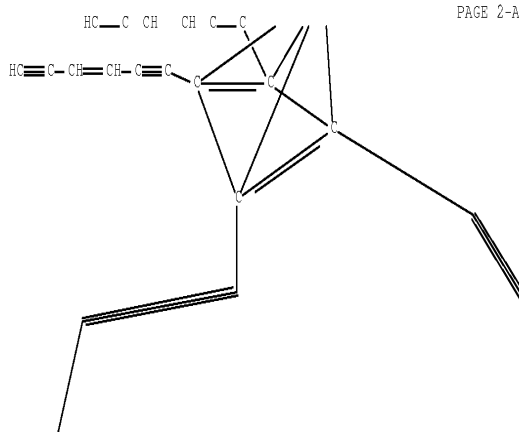
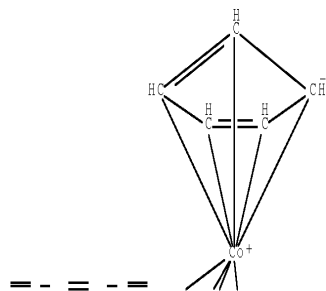
L8 ANSWER 28 OF 39 CAPLUS COPYRIGHT 2009 ACS on STN  
 ACCESSION NUMBER: 2001:318816 CAPLUS [Full-text](#)  
 DOCUMENT NUMBER: 135:92741  
 TITLE: Concave butterfly-shaped organometallic hydrocarbons?  
 AUTHOR(S): Laskoski, Matthew; Roidl, Gaby; Smith, Mark D.; Bunz, Uwe H. F.  
 CORPORATE SOURCE: Department of Chemistry and Biochemistry, The University of South Carolina, Columbia, SC, 29208, USA  
 SOURCE: Angewandte Chemie, International Edition (2001), 40(8), 1460-1463  
 CODEN: ACIEF5; ISSN: 1433-7851  
 PUBLISHER: Wiley-VCH Verlag GmbH  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 OTHER SOURCE(S): CASREACT 135:92741  
 GI



AB The preparation of title novel large concave organometallic hydrocarbon with a central tetraethynylcyclobutadiene(cyclopentadienylcobalt) core, e.g. I, starting from tetraalkynylcyclobutadiene cobalt complex in five steps is described. The crystal structure of I was determined  
 IT 349453-21-0P  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
 (preparation and cyclization of)  
 RN 349453-21-0 CAPLUS  
 CN Cobalt, ( $\eta^5$ -2,4-cyclopentadien-1-yl)[(1,2,2a,18a- $\eta$ )-3,4,9,10,11,12,17,18-octadehydro-7,14-bis(1,1-dimethylethyl)-1,2-di-(3Z)-3-hexene-1,5-diynyl]dibenzo[a,i]cyclobuta[e]cyclotetradecene)- (9CI) (CA INDEX NAME)

OS.CITING REF COUNT: 27 THERE ARE 27 CAPLUS RECORDS THAT CITE THIS RECORD (28 CITINGS)  
 REFERENCE COUNT: 37 THERE ARE 37 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

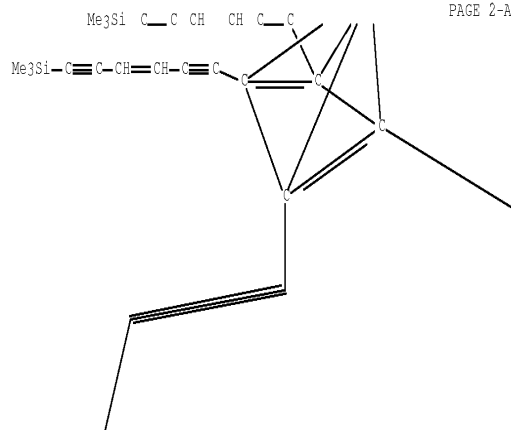
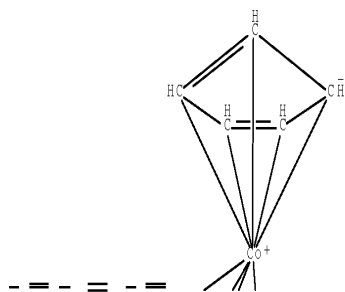




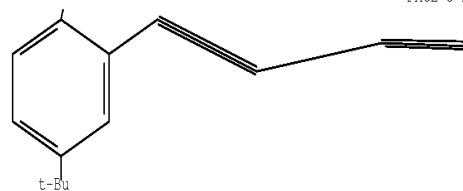
IT 343453-20-3P  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT  
 (Reactant or reagent)  
 (preparation and desilylation of)  
 RN 349453-20-9 CAPLUS  
 CN Cobalt, (η<sup>5</sup>-2,4-cyclopentadien-1-yl)[[(1,2,2a,18a-η)-  
 3,4,9,10,11,12,17,18-octadehydro-7,14-bis(1,1-  
 dimethylethyl)dibenzo[a,i]cyclobuta[e]cyclotetradecene-1,2-diyl]di-(3Z)-3-



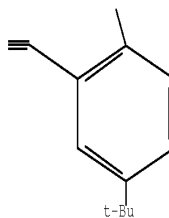
PAGE 1-A



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PAGE 3-A



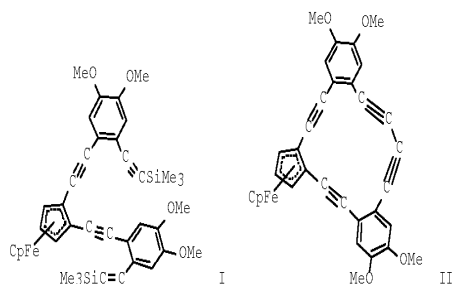
PAGE 3-B

OS.CITING REF COUNT: 21 THERE ARE 21 CAPLUS RECORDS THAT CITE THIS RECORD (21 CITINGS)  
 REFERENCE COUNT: 31 THERE ARE 31 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

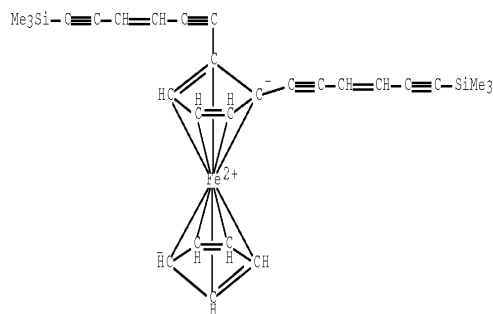
L8 ANSWER 29 OF 39 CAPLUS COPYRIGHT 2009 ACS on STN  
 ACCESSION NUMBER: 2001:295307 CAPLUS Full-text  
 DOCUMENT NUMBER: 135:107433



TITLE: Is ferrocene more aromatic than benzene?  
 AUTHOR(S): Laskoski, Matthew; Steffen, Winfried; Smith, Mark D.; Bunz, Uwe H. F.  
 CORPORATE SOURCE: Department of Chemistry and Biochemistry, The University of South Carolina, Columbia, SC, 29208, USA  
 SOURCE: Chemical Communications (Cambridge, United Kingdom) (2001), (8), 691-692  
 CODEN: CHCOFS; ISSN: 1359-7345  
 PUBLISHER: Royal Society of Chemistry  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 OTHER SOURCE(S): CASREACT 135:107433  
 GI

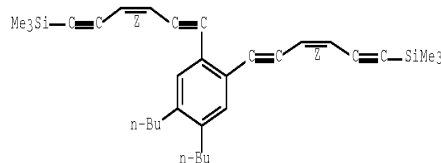


AB A combination of Pd-catalyzed arene-alkynyl couplings and Cu(OAc)<sub>2</sub>-promoted internal alkyne dimerization furnishes novel ferrocene-based dehydroannulenes in high yield. Thus, palladium-copper catalyzed coupling of 1,2-diethynylferrocene 1-I-2,3-(MeO)<sub>2</sub>C<sub>6</sub>H<sub>2</sub>C.tplbond.CSiMe<sub>3</sub> gave 30% tetrayne I which on K<sub>2</sub>CO<sub>3</sub>/MeOH mediated desilylation followed by cyclization with Cu(OAc)<sub>2</sub>/MeCN gave 49% dehydroannulene II.  
 IT 350586-85-5P 350586-94-6P  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
 (preparation, desilylation, and sequential copper catalyzed cyclization of)  
 RN 350586-85-5 CAPLUS  
 CN Ferrocene, 1,2-bis[(3Z)-6-(trimethylsilyl)-3-hexene-1,5-diynyl]- (9CI)  
 (CA INDEX NAME)



RN 350586-94-6 CAPLUS  
 CN Silane, [(4,5-dibutyl-1,2-phenylene)di-(3Z)-3-hexene-1,5-diyne-6,1-diyl]bis(trimethyl- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



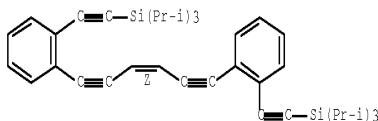
OS.CITING REF COUNT: 28 THERE ARE 28 CAPLUS RECORDS THAT CITE THIS RECORD (28 CITINGS)  
 REFERENCE COUNT: 16 THERE ARE 16 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 30 OF 39 CAPLUS COPYRIGHT 2009 ACS on STN  
 ACCESSION NUMBER: 2000:832492 CAPLUS [Full-text](#)  
 DOCUMENT NUMBER: 134:310920  
 TITLE: Bis(enediynes) Macrocycles: Synthesis, Reactivity, and Structural Analysis  
 AUTHOR(S): Blanchette, H. S.; Brand, S. C.; Naruse, H.; Weakley, T. J. R.; Haley, M. M.  
 CORPORATE SOURCE: Department of Chemistry, University of Oregon, Eugene, OR, 97403-1253, USA  
 SOURCE: Tetrahedron (2000), 56(49), 9581-9588  
 CODEN: TETRAB; ISSN: 0040-4020  
 PUBLISHER: Elsevier Science Ltd.  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 OTHER SOURCE(S): CASREACT 134:310920  
 AB The authors describe the syntheses of five macrocycles possessing two enediyne warheads, along with the structural and thermal analyses of these bis(enediynes) compds. The solid-state packing of one of the compds. suggests the possibility for the mol. to undergo a topochem. diacetylene polymerization  
 IT 335378-20-6P 335378-30-6P  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT



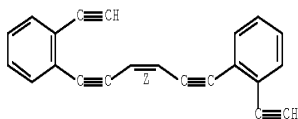
(Reactant or reagent)  
 (preparation of bis(enediynes) macrocycles)  
 RN 335378-20-6 CAPLUS  
 CN Silane, [(3Z)-3-hexene-1,5-diyne-1,6-diylbis(2,1-phenylene-2,1-ethynediyl)]bis[tris(1-methylethyl)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



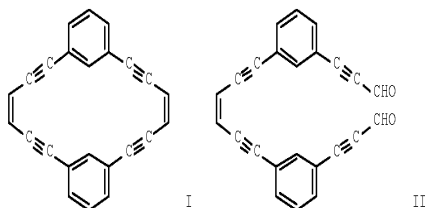
RN 335378-30-8 CAPLUS  
 CN Benzene, 1,1'-(3Z)-3-hexene-1,5-diyne-1,6-diylbis[2-ethynyl- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



OS.CITING REF COUNT: 19 THERE ARE 19 CAPLUS RECORDS THAT CITE THIS RECORD (20 CITINGS)  
 REFERENCE COUNT: 37 THERE ARE 37 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 31 OF 39 CAPLUS COPYRIGHT 2009 ACS on STN  
 ACCESSION NUMBER: 2000:767122 CAPLUS [Full-text](#)  
 DOCUMENT NUMBER: 134:71381  
 TITLE: Synthesis and structure of a new [6.6]metacyclophane with enediynes bridges  
 AUTHOR(S): Srinivasan, Manivannan; Sankararaman, Sethuraman; Dix, Ina; Jones, Peter G.  
 CORPORATE SOURCE: Department of Chemistry, Indian Institute of Technology, Madras, 600 036, India  
 SOURCE: Organic Letters (2000), 2(24), 3849-3851  
 CODEN: ORLEF7; ISSN: 1523-7060  
 PUBLISHER: American Chemical Society  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 OTHER SOURCE(S): CASREACT 134:71381  
 GI



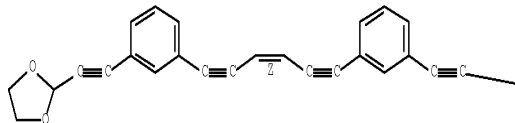
AB Synthesis and structure of a novel [6.6]metacyclophane with enediynes bridges I is reported. I was prepared by reacting 1,3-diethynylbenzene with EtMgBr/THF and DMF to give the monoaldehyde. The monoaldehyde was subsequently converted to the acetal, coupled with ClCH:CHCl to give bis-acetal, which was hydrolyzed to the dialdehyde II. II underwent McMurry coupling using TiCl3 and Zn-Cu couple in DME to give I in 69% yield.

IT 315716-90-6P 315716-91-3P  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
 (preparation and crystal structure of metacyclophane with enediynes bridges)

RN 315716-90-6 CAPLUS  
 CN 1,3-Dioxolane, 2,2'-[(3Z)-3-hexene-1,5-diyne-1,6-diylbis(3,1-phenylene-2,1-ethynediyl)]bis- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

PAGE 1-A



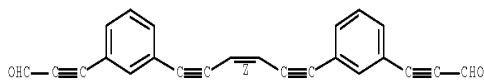
PAGE 1-B



RN 315716-91-7 CAPLUS  
 CN 2-Propynal, 3,3'-[(3Z)-3-hexene-1,5-diyne-1,6-diylbis(3,1-phenylene)]bis- (9CI) (CA INDEX NAME)

Double bond geometry as shown.





OS.CITING REF COUNT: 18 THERE ARE 18 CAPLUS RECORDS THAT CITE THIS RECORD (18 CITINGS)

REFERENCE COUNT: 31 THERE ARE 31 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 32 OF 39 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1999:625317 CAPLUS Full-text

DOCUMENT NUMBER: 131:337377

TITLE: Modulation of  $\pi$ -electron conjugation in oligo(triacetylene) chromophores by incorporation of a central spacer

AUTHOR(S): Martin, Rainer E.; Wytko, Jennifer A.; Diederich, Francois; Boudon, Corinne; Gisselbrecht, Jean-Paul; Gross, Maurice

CORPORATE SOURCE: Laboratorium fur Organische Chemie, ETH-Zentrum, Zurich, CH-8092, Germany

SOURCE: Helvetica Chimica Acta (1999), 82(9), 1470-1485  
CODEN: HCACAV; ISSN: 0018-019X

PUBLISHER: Verlag Helvetica Chimica Acta

DOCUMENT TYPE: Journal

LANGUAGE: English

AB A series of trimeric hybrid oligomers was prepared by insertion of different hetero-spacers between two (E)-hex-3-ene-1,5-diyne (E = 1,2-diethynylethene, DEE) moieties, and the optical and electrochem. properties of the resulting  $\pi$ -conjugated materials were compared to those of the DEE dimer and trimer, which formally contain a DEE moiety as homo-spacer. The hetero-spacers were: benzenoid (phenylene, naphthalene, biphenylene, anthracene),  $\pi$ -electron-deficient (pyrazine, pyridine) and  $\pi$ -electron-rich (thiophene, furan) aromatic rings, and trans-Pt(PtEt3)2. The hybrid oligomers were synthesized using the method of K. Sonogashira et al. (1978), i.e., cross-coupling between mono-deprotected DEE and the appropriately bis-functionalized spacer. UV/VIS data revealed that the majority of the hetero-spacers were less effective than the homo-spacer DEE in facilitating  $\pi$ -electron delocalization along the linearly conjugated oligomeric backbone. With increasing degree of benzenoid aromaticity in the hetero-spacer, the electronic communication between the terminal DEE moieties in the hybrid oligomers was reduced. As a remarkable exception, a large bathochromic shift of the longest-wavelength absorption maximum, which is indicative of enhanced  $\pi$ -electron delocalization, was obtained upon introducing an anthracene-9,10-diyl moiety as hetero-spacer. Electrochem. studies by cyclic and steady-state voltammetry confirmed the limited extent of  $\pi$ -electron delocalization in the majority of the hybrid oligomers. The fluorescence properties of many of the DEE hybrid materials were dramatically enhanced upon incorporation of the heterospacers. The heterocyclic derivs. containing pyridine, pyrazine, or thiophene spacers, resp., displayed a strong fluorescence emission, demonstrating the value of combining repeat units to modulate oligomeric and polymeric properties. The pyridine derivative provided an interesting example of a mol. system, in which both the electronic absorption and emission characteristics can be reversibly switched as a function of pH.

IT 249616-79-3P, 4-Bis[(E)-3,4-bis[[tert-butyl]dimethylsilyloxy]methyl]-6-(trimethylsilyl)-hex-3-ene-1,5-diynyl]benzene 249616-82-8P,

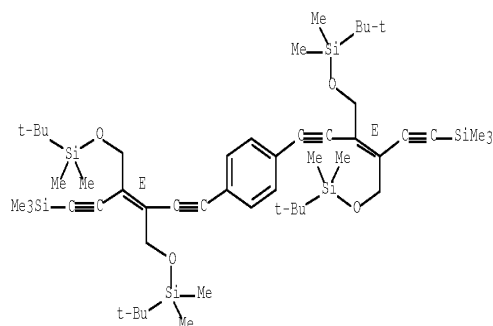
2,6-Bis[(E)-3,4-bis[[tert-butyl]dimethylsilyloxy]methyl]-6-(trimethylsilyl)-hex-3-ene-1,5-diynyl]naphthalene 249616-83-3P, 9,10-Bis[(E)-3,4-bis[[tert-butyl]dimethylsilyloxy]methyl]-6-(trimethylsilyl)-hex-3-ene-1,5-diynyl]anthracene 249616-84-0P 249616-87-3P, 1,4-Bis[(E)-3,4-bis[[tert-butyl]dimethylsilyloxy]methyl]-6-(trimethylsilyl)-hex-3-ene-1,5-diynyl]-2,3,5,6-tetramethylbenzene 249616-88-4P 249616-89-5P, 2,5-Bis[(E)-3,4-bis[[tert-butyl]dimethylsilyloxy]methyl]-6-(trimethylsilyl)-hex-3-ene-1,5-diynyl]pyrazine 249616-90-8P 249616-91-9P, 2,5-Bis[(E)-3,4-bis[[tert-butyl]dimethylsilyloxy]methyl]-6-(trimethylsilyl)-hex-3-ene-1,5-diynyl]furan

RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation) (preparation and modulation of  $\pi$ -electron conjugation in oligoacetylene chromophores by central spacer with variable electron d.)

RN 249616-79-3 CAPLUS

CN 4,9-Dioxa-3,10-disiladodec-6-ene, 6,6'-(1,4-phenylenedi-2,1-ethynediyl)bis[2,2,3,3,10,10,11,11-octamethyl-7-[(trimethylsilyl)ethynyl]-, (6E,6'E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



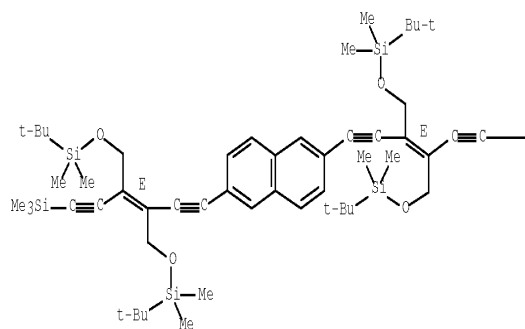
RN 249616-82-8 CAPLUS

CN 4,9-Dioxa-3,10-disiladodec-6-ene, 6,6'-(2,6-naphthalenediyl)-2,1-ethynediyl]bis[2,2,3,3,10,10,11,11-octamethyl-7-[(trimethylsilyl)ethynyl]-, (6E,6'E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



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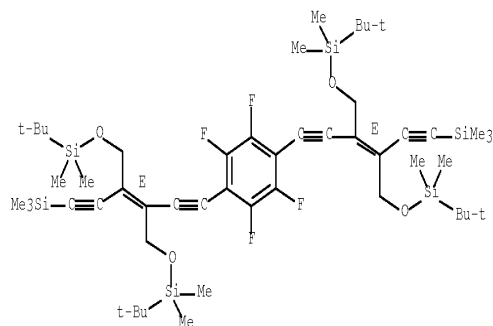
PAGE 1-B

—SiMe<sub>3</sub>

RN 249616-84-0 CAPLUS

CN 4,9-Dioxo-3,10-disiladodec-6-ene, 6,6'-[(2,3,5,6-tetrafluoro-1,4-phenylene)di-2,1-ethynediyl]bis[2,2,3,3,10,10,11,11-octamethyl-7-[(trimethylsilyl)ethynyl]-, (6E,6'E)- (9CI) (CA INDEX NAME)

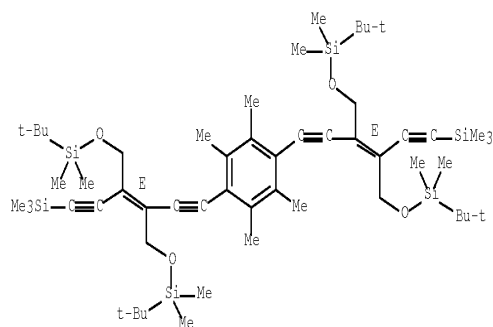
Double bond geometry as shown.



RN 249616-87-3 CAPLUS

CN 4,9-Dioxo-3,10-disiladodec-6-ene, 6,6'-[(2,3,5,6-tetramethyl-1,4-phenylene)di-2,1-ethynediyl]bis[2,2,3,3,10,10,11,11-octamethyl-7-[(trimethylsilyl)ethynyl]-, (6E,6'E)- (9CI) (CA INDEX NAME)

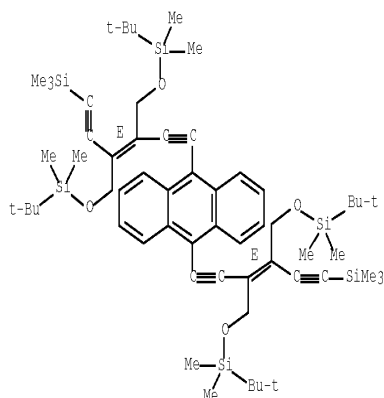
Double bond geometry as shown.



RN 249616-83-9 CAPLUS

CN 4,9-Dioxo-3,10-disiladodec-6-ene, 6,6'-[(9,10-anthracenediyl)di-2,1-ethynediyl]bis[2,2,3,3,10,10,11,11-octamethyl-7-[(trimethylsilyl)ethynyl]-, (6E,6'E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

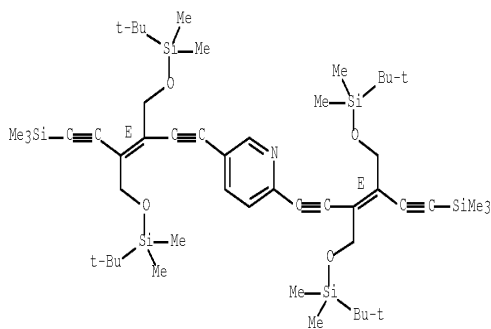


RN 249616-88-4 CAPLUS

CN Pyridine, 2,5-bis[(3E)-3,4-bis[[[(1,1-dimethylethyl)dimethylsilyl]oxy]methyl]-6-(trimethylsilyl)-3-hexene-1,5-diyn-1-yl]- (CA INDEX NAME)

Double bond geometry as shown.

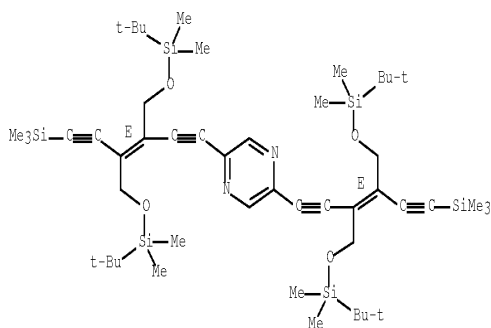




RN 249616-89-5 CAPLUS

CN Pyrazine, 2,5-bis[(3E)-3,4-bis[[[(1,1-dimethylethyl)dimethylsilyl]oxy]methyl]-6-(trimethylsilyl)-3-hexene-1,5-diyn-1-yl]- (CA INDEX NAME)

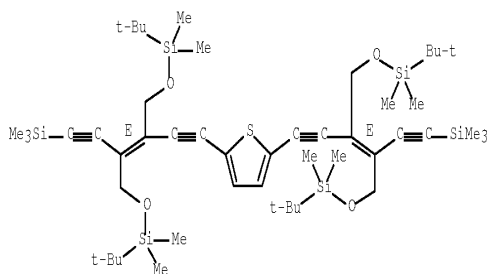
Double bond geometry as shown.



RN 249616-90-8 CAPLUS

CN 4,9-Dioxa-3,10-disiladodec-6-ene, 6,6'-(2,5-thiophenediyl)-2,1-ethynediyl]bis[2,2,3,3,10,10,11,11-octamethyl-7-[(trimethylsilyl)ethynyl]-, (6E,6'E)- (9CI) (CA INDEX NAME)

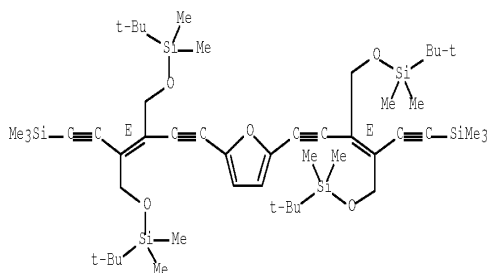
Double bond geometry as shown.



RN 249616-91-9 CAPLUS

CN 4,9-Dioxa-3,10-disiladodec-6-ene, 6,6'-(2,5-furandiyl)-2,1-ethynediyl]bis[2,2,3,3,10,10,11,11-octamethyl-7-[(trimethylsilyl)ethynyl]-, (6E,6'E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



OS.CITING REF COUNT: 29 THERE ARE 29 CAPLUS RECORDS THAT CITE THIS RECORD (29 CITINGS)

REFERENCE COUNT: 69 THERE ARE 69 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 33 OF 39 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1998:756297 CAPLUS [Full-text](#)

DOCUMENT NUMBER: 130:118607

TITLE: Porphyrin-[(E)-1,2-diethynylethene] scaffolding. Synthesis and optical and electrochemical properties of multiananometer-sized porphyrin arrays

AUTHOR(S): Wytko, Jennifer; Berl, Volker; McLaughlin, Mark; Tykwinski, Rik R.; Schreiber, Martin; Diederich, Francois; Boudon, Corinne; Gisselbrecht, Jean-Paul; Gross, Maurice

CORPORATE SOURCE: Laboratorium Organische Chemie, ETH-Zentrum, Zurich, CH-8092, Switz.

SOURCE: Helvetica Chimica Acta (1998), 81(11), 1964-1977

CODEN: HCACAV; ISSN: 0018-019X

PUBLISHER: Verlag Helvetica Chimica Acta AG

DOCUMENT TYPE: Journal



\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

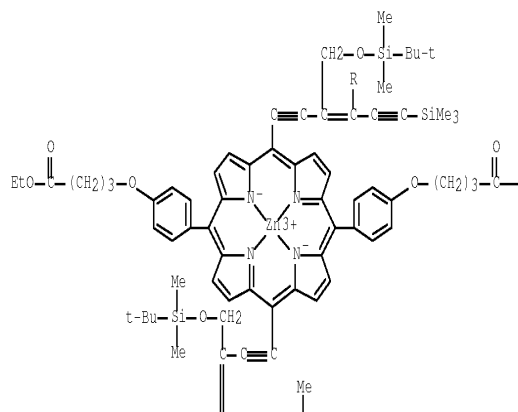
AB Two series of linearly conjugated hybrid materials, consisting of (E)-1,2-diethynylethene (DEE; hex-3-ene-1,5-diyne) and Zn(II) porphyrin components, were prepared by Pd0-catalyzed cross-coupling reactions. In 1 series, 1 or 2 DEE substituents were introduced into the meso-positions of the Zn(II) porphyrins, leading from Zn 5,15-bis((ethoxycarbonyl)propoxy)phenylporphinate (I) to I and II (n = 1; R = SiMe2tBu). The second series contains the linearly  $\pi$ -conjugated mol. rods III (n = 1-3) that span a length range from 23 Å for III (n = 1) to 53 Å for III (n = 3). The larger rods III (n = 2 and 3) consist of 2 or 3 porphyrin moieties, resp., that are bridged at the meso-positions by trans-enediynediyl (hex-3-ene-1,5-diyne-1,6-diyl) linkers. The UV/VIS spectra in the series I, II, and III (n = 1) showed a strong bathochromic shift of both Soret and Q bands of the Zn(II) porphyrin as a result of the addition of DEE substituents. Upon changing from I to II, the Q band was further bathochromically shifted, whereas the Soret band remained nearly at the same position but became broadened and displayed a shoulder on the lower-wavelength edge as a result of excitonic coupling. The close resemblance between the UV/Vis spectra of III (n = 2 and 3) suggests that saturation of the optical properties in the oligomeric series already occurs at the stage of dimeric III (n = 2). Stationary voltammetric investigations showed that the DEE substituents act as strong electron acceptors which induce large anodic shifts in the 1st reduction potential upon changing from I to II ( $\Delta E = 190$  mV) and to III (n = 1) ( $\Delta E = 340$  mV). Increasing the number of porphyrin moieties upon changing from III (n = 1) to III (n = 2) had no effect on the 1st reduction potential yet the 1st oxidation potential was substantially lowered ( $\Delta E = 110$  mV). Large differences in the potentials for 1-electron oxidation of the 2 porphyrin moieties in III (n = 2) ( $\Delta E = 200$  mV) confirmed the existence of substantial electronic communication between the 2 macrocycles across the trans-enediynediyl bridge.

IT 219483-26-3 219483-27-3  
RL: FMU (Formation, unclassified); PRP (Properties); FORM (Formation, nonpreparative)

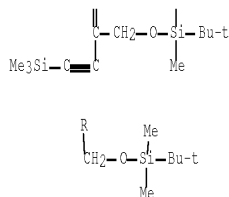
(elec. potential of couple containing)

RN 219483-26-8 CAPLUS

CN Zinc(1+), [[diethyl 4,4'-[[10,20-bis[(3E)-3,4-bis[[[(1,1-dimethylethyl)dimethylsilyl]oxy]methyl]-6-(trimethylsilyl)-3-hexene-1,4-diynyl]-21H,23H-porphine-5,15-diyl-  
K21,K22,K23,K24]bis(4,1-phenyleneoxy)]bis[butanoato]](2-)]-, (SP-4-1)- (9CI) (CA INDEX NAME)



—OEt

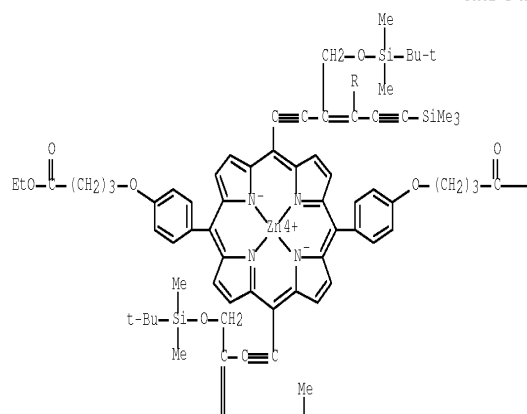


RN 219483-27-9 CAPLUS

CN Zinc(2+), [[diethyl 4,4'-[[10,20-bis[(3E)-3,4-bis[[[(1,1-dimethylethyl)dimethylsilyl]oxy]methyl]-6-(trimethylsilyl)-3-hexene-1,4-diynyl]-21H,23H-porphine-5,15-diyl-  
K21,K22,K23,K24]bis(4,1-phenyleneoxy)]bis[butanoato]](2-)]-, (SP-4-1)- (9CI) (CA INDEX NAME)



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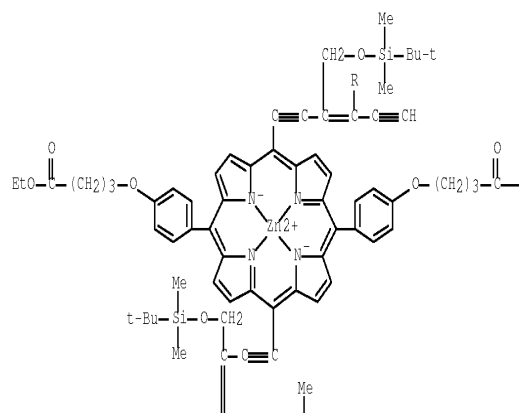


PAGE 1-B

—OEt

porphine-5,15-diyl-κN21,κN22,κN23,κN24]bis(4,1-phenyleneoxy)]bis[butanoato]](2-)]-, (SP-4-1)- (9CI) (CA INDEX NAME)

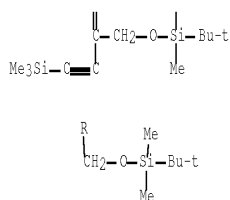
PAGE 1-A



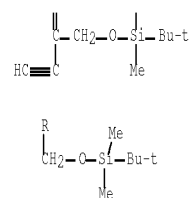
PAGE 1-B

—OEt

PAGE 2-A



PAGE 2-A



IT 219483-13-3P  
 RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
 (preparation of reactant for preparation zinc porphyrin diethynylethene monomeric, dimeric, and trimeric complexes and NMR)  
 RN 219483-18-8 CAPLUS  
 CN Zinc, [[diethyl 4,4'-[[[10,20-bis[(3E)-3,4-bis[[[(1,1-dimethylethyl)dimethylsilyl]oxy]methyl]-3-hexene-1,5-diynyl]-21H,23H-

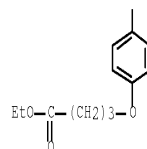
IT 219483-13-3P  
 RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
 (preparation, UV spectra, electrochem. redox behavior and conversion to



trinuclear complex and NMR)

RN 219483-19-9 CAPLUS

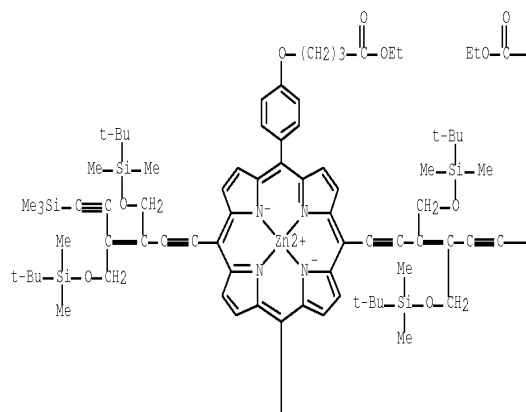
CN Zinc, [ $\mu$ -[[[tetraethyl 4,4',4'',4'''-[[[(3E)-3,4-bis[[[(1,1-dimethylethyl)dimethylsilyl]oxy)methyl]-3-hexene-1,5-diyne-1,6-diyl]bis[[20-[(3E)-3,4-bis[[[(1,1-dimethylethyl)dimethylsilyl]oxy)methyl]-6-(trimethylsilyl)-3-hexene-1,5-diynyl]-21H,23H-porphine-10,5,15-triyl- $\kappa$ N21, $\kappa$ N22, $\kappa$ N23, $\kappa$ N24]-4,1-phenyleneoxy]]tetrakis[butanoato]](4-)]di- (9CI) (CA INDEX NAME)



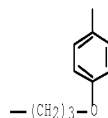
PAGE 2-A



PAGE 1-A



PAGE 2-B



IT 219483-15-5P

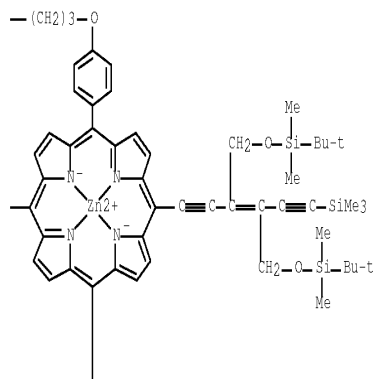
RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation, UV spectra, electrochem. redox behavior, and deprotection and NMR)

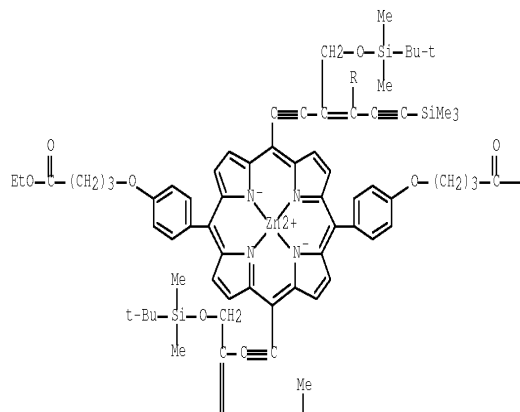
RN 219483-15-5 CAPLUS

CN Zinc, [[diethyl 4,4'-[[[10,20-bis[(3E)-3,4-bis[[[(1,1-dimethylethyl)dimethylsilyl]oxy)methyl]-6-(trimethylsilyl)-3-hexene-1,4-diynyl]-21H,23H-porphine-5,15-diyl- $\kappa$ N21, $\kappa$ N22, $\kappa$ N23, $\kappa$ N24]bis(4,1-phenyleneoxy)]bis[butanoato]](2-)]-, (SP-4-1)- (9CI) (CA INDEX NAME)

PAGE 1-B

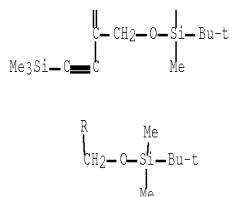
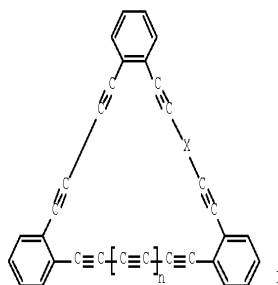


PAGE 1-A





—OEt



OS.CITING REF COUNT: 45 THERE ARE 45 CAPLUS RECORDS THAT CITE THIS RECORD (45 CITINGS)

REFERENCE COUNT: 64 THERE ARE 64 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 34 OF 39 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1998:606810 CAPLUS [Full-text](#)

DOCUMENT NUMBER: 129:302407

ORIGINAL REFERENCE NO.: 129:61683a,61686a

TITLE: Synthesis of expanded planar dehydrobenzoannulenes: weakly diatropic, weakly paratropic, or atropic?

AUTHOR(S): Wan, W. Brad; Kimball, David B.; Haley, Michael M.

CORPORATE SOURCE: Department of Chemistry, University of Oregon, Oregon, 97403-1253, USA

SOURCE: Tetrahedron Letters (1998), 39(38), 6795-6798

CODEN: TELEAY; ISSN: 0040-4039

PUBLISHER: Elsevier Science Ltd.

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 129:302407

GI

AB Use of a Cu/Pd cross-coupling strategy has led to the synthesis of the first dehydrobenzoannulenes I [X = C.tplbond.C, (E)-CH:CH; n = 0,1] containing triacetylenic linkages. NMR studies of these macrocycles and comparison with other known systems indicate that, in spite of their large size and extensive benzannulation, dehydrobenzoannulenes possess weak induced ring currents.

IT 214628-16-78 214628-17-38 214628-18-39

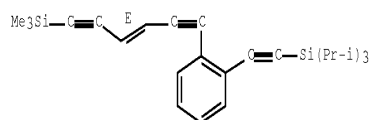
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of expanded planar dehydrobenzoannulenes with triacetylenic linkages)

RN 214628-16-7 CAPLUS

CN Benzene, 1-[(3E)-6-(trimethylsilyl)-3-hexene-1,5-diyn-1-yl]-2-[2-[tris(1-methylethyl)silyl]ethynyl]- (CA INDEX NAME)

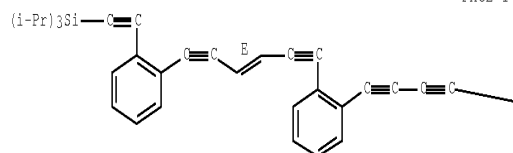
Double bond geometry as shown.



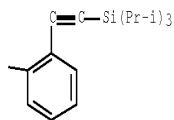
RN 214628-17-8 CAPLUS

CN Silane, tris(1-methylethyl)[[2-[(3E)-6-[2-[4-[2-[tris(1-methylethyl)silyl]ethynyl]phenyl]-1,3-butadiynyl]phenyl]-3-hexene-1,5-diynyl]phenyl]ethynyl]- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



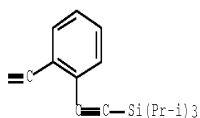
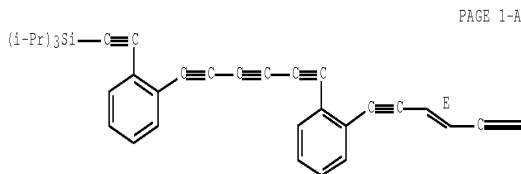




RN 214628-18-9 CAPLUS

CN Silane, tris(1-methylethyl)[[2-[6-[2-[(3E)-6-[2-[[tris(1-methylethyl)silyl]ethynyl]phenyl]-3-hexene-1,5-diynyl]phenyl]-1,3,5-hexatriynyl]phenyl]ethynyl]- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



OS.CITING REF COUNT: 25 THERE ARE 25 CAPLUS RECORDS THAT CITE THIS RECORD (26 CITINGS)

REFERENCE COUNT: 18 THERE ARE 18 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 35 OF 39 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1994:680471 CAPLUS [Full-text](#)

DOCUMENT NUMBER: 121:280471

ORIGINAL REFERENCE NO.: 121:51203a,51206a

TITLE: Preparation of dynemicin analogs as bactericides and antitumor agents

INVENTOR(S): Smith, Adrian L.; Hwang, Chan Kou; Wenderborn, Sebastian V.; Nicolaou, Kyriacos C.; Schreiner, Erwin P.; Stahl, Wilhelm; Dai, Wei Min; Maligres, Peter E.; Suzuki, Toshio

PATENT ASSIGNEE(S): Scripps Research Institute, USA

SOURCE: U.S., 114 pp. Cont.-in-part of U.S.Ser. No. 886,984,abandoned.

CODEN: USXXAM

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 5

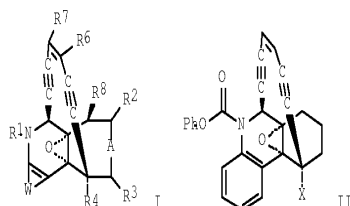
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 5281710	A	19940125	US 1992-939104	19920901
US 5276159	A	19940104	US 1992-886984	19920521
US 5500432	A	19960319	US 1993-46626	19930414
WO 9323046	A1	19931125	WO 1993-US4708	19930518
W: AU, CA, FI, JP, NO				
RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
AU 9343807	A	19931213	AU 1993-43807	19930518
AU 680418	B2	19970731		
EP 641207	A1	19950308	EP 1993-913966	19930518
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, MC, NL, PT, SE				
JP 07508037	T	19950907	JP 1994-503816	19930518
US 5527805	A	19960618	US 1994-184580	19940121
FI 9405427	A	19950118	FI 1994-5427	19941118
NO 9404429	A	19950123	NO 1994-4429	19941118
PRIORITY APPLN. INFO.:				
			US 1990-562269	B2 19900801
			US 1991-673199	B2 19910321
			US 1991-734613	B2 19910723
			US 1991-788225	B2 19911105
			US 1992-886984	B2 19920521
			US 1992-939104	A2 19920901
			WO 1993-US4708	A 19930518

ASSIGNMENT HISTORY FOR US PATENT AVAILABLE IN LSUS DISPLAY FORMAT

OTHER SOURCE(S): MARPAT 121:280471

GI



AB The title compds. I [A = double or single bond; R1 = H, alkyl, phenoxycarbonyl, etc.; R2 = H, carboxyl, hydroxylmethyl, etc.; R3 = H, alkoxy; R4 = H, hydroxyl, alkoxy, etc.; R6 and R7 are each H or together with the intervening vinylene group form a one, two or three fused aromatic six-membered ring system; W together with the bonded, intervening, vinylene group (i.e., the unsatd. carbon atoms bonded to W) forms a substituted aromatic hydrocarbyl ring system containing 1, 2, or 3 six-membered rings such that said fused ring compound contains 3, 4, or 5 fused 6-membered rings all but two of which rings are aromatic, and in which that aromatic hydrocarbyl ring



system, W, is joined [a,b] to the structure shown; R8 = H, or Me; a proviso is given] are prepared Title compound II (X = OH) (preparation given) in vitro exhibited IC50 of 6.3 x 10<sup>-6</sup> M against a variety of cancer cell lines. II (X = H) in vitro exhibited IC50 of 5.0 x 10<sup>-6</sup> M against a variety of cancer cell lines.

IT 144127-80-0P 144127-81-1P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

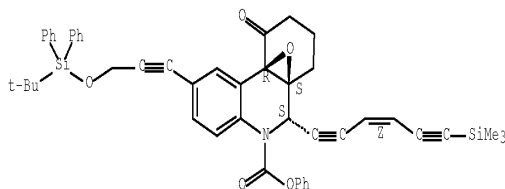
(preparation and reaction of, in preparation of bactericide and antitumor agent)

RN 144127-80-0 CAPLUS

CN 6a,10a-Epoxyphenanthridine-5(6H)-carboxylic acid, 2-[3-[[[1,1-dimethylethyl)diphenylsilyl]oxy]-1-propynyl]-7,8,9,10-tetrahydro-10-oxo-6-[6-(trimethylsilyl)-3-hexene-1,5-diynyl]-, phenyl ester, [6 $\alpha$ (Z),6 $\alpha$  $\beta$ ,10 $\alpha$  $\beta$ ]- (9CI) (CA INDEX NAME)

Relative stereochemistry.

Double bond geometry as shown.

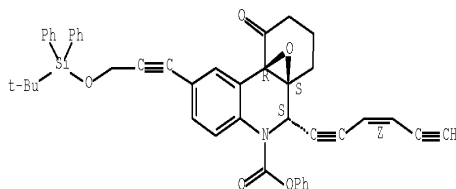


RN 144127-81-1 CAPLUS

CN 6a,10a-Epoxyphenanthridine-5(6H)-carboxylic acid, 2-[3-[[[1,1-dimethylethyl)diphenylsilyl]oxy]-1-propynyl]-6-(3-hexene-1,5-diynyl)-7,8,9,10-tetrahydro-10-oxo-, phenyl ester, [6 $\alpha$ (Z),6 $\alpha$  $\beta$ ,10 $\alpha$  $\beta$ ]- (9CI) (CA INDEX NAME)

Relative stereochemistry.

Double bond geometry as shown.



OS.CITING REF COUNT: 4 THERE ARE 4 CAPLUS RECORDS THAT CITE THIS RECORD (4 CITINGS)

REFERENCE COUNT: 13 THERE ARE 13 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 36 OF 39 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1994:680470 CAPLUS Full-text

DOCUMENT NUMBER: 121:280470

ORIGINAL REFERENCE NO.: 121:51202h,51203a

TITLE: Preparation of dymecicin analogs as DNA binding, antibiotic, and antitumor agents.

INVENTOR(S): Smith, Adrian L.; Hwang, Chan Kou; Wendeborn, Sebastian V.; Nicolaou, Kyriacos C.; Schreiner, Erwin P.; Stahl, Wilhelm; Dai, Wei Min; Maligres, Peter E.; Suzuki, Toshio

PATENT ASSIGNEE(S): Scripps Research Institute, USA

SOURCE: U.S., 109 pp. Cont.-in-part of U.S. Ser. No. 788,225.

CODEN: USXXAM

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 5

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 5276159	A	19940104	US 1992-886984	19920521
US 5281710	A	19940125	US 1992-939104	19920901
US 5500432	A	19960319	US 1993-46626	19930414
WO 9323046	A1	19931125	WO 1993-US4708	19930518
W: AU, CA, FI, JP, NO				
RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
AU 9343807	A	19931213	AU 1993-43807	19930518
AU 680418	B2	19970731		
EP 641207	A1	19950308	EP 1993-913966	19930518
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, MC, NL, PT, SE				
JP 07508037	T	19950907	JP 1994-503816	19930518
US 5527805	A	19960618	US 1994-184580	19940121
FI 9405427	A	19950118	FI 1994-5427	19941118
NO 9404429	A	19950123	NO 1994-4429	19941118
PRIORITY APPLN. INFO.:			US 1990-562269	B2 19900801
			US 1991-673199	B2 19910321
			US 1991-734613	B2 19910723
			US 1991-788225	A2 19911105
			US 1992-886984	B2 19920521
			US 1992-939104	A2 19920901
			WO 1993-US4708	A 19930518

ASSIGNMENT HISTORY FOR US PATENT AVAILABLE IN LSUS DISPLAY FORMAT

OTHER SOURCE(S): MARPAT 121:280470

GI

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

AB Title compds. [I; R1 = H, alkyl, PhO2C, PhCH2O2C, 9-fluorenylmethoxycarbonyl, o-nitrobenzyloxycarbonyl, (substituted) alkoxycarbonyl; R2 = H, CO2H, CH2OH, carbonyloxyalkyl; R3 = H, alkoxy; R4 = H, OH, alkoxy, oxyacetic acid, oxyacetic hydrocarbyl or benzyl ester, oxyacetic amide, acyloxy, etc.; R6, R7 = H; R6R7 = atoms to form a 1, 2, or 3-fused aromatic 6-membered ring system; R8 = H, Me, with provisos; A = double or single bond; W = atoms to form an aromatic hydrocarbyl ring system containing 1, 2, or 3 six-membered rings such that the fused ring compound contains 3, 4, or 5 fused rings, all but 2 of which are aromatic], were prepared Chimeric compds. having the fused ring system compound as an aglycon bonded to (i) a sugar moiety as the oligosaccharide portion or (ii) a monoclonal antibody or antibody combining site portion thereof that immunoreacts with target tumor cells are also



disclosed. Thus, title compound III (preparable via claimed compound II) inhibited Molt-4 T-cell leukemia with IC50 = 2.0 + 10-14 M; III was 1-8 orders of magnitude more active against tumor cells than against normal cells. I structure-activity relationships are discussed.

IT 144127-31-1F

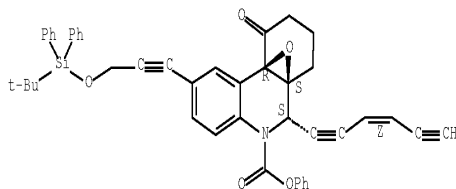
RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation of, as DNA binding, antibiotic, and antitumor agent)

RN 144127-81-1 CAPLUS

CN 6a,10a-Epoxyphenanthridine-5(6H)-carboxylic acid,  
2-[3-[[[1,1-dimethylethyl]diphenylsilyl]oxy]-1-propynyl]-6-(3-hexene-1,5-diy-  
nyl)-7,8,9,10-tetrahydro-10-oxo-, phenyl ester,  
[6 $\alpha$ (Z),6 $\alpha$  $\beta$ ,10 $\alpha$  $\beta$ ]- (9CI) (CA INDEX NAME)

Relative stereochemistry.

Double bond geometry as shown.



IT 144127-80-0F

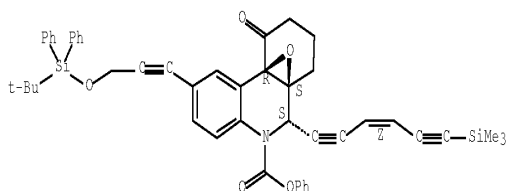
RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation of, as intermediate for DNA binding, antibiotic, and antitumor  
dymenicin analog)

RN 144127-80-0 CAPLUS

CN 6a,10a-Epoxyphenanthridine-5(6H)-carboxylic acid,  
2-[3-[[[1,1-dimethylethyl]diphenylsilyl]oxy]-1-propynyl]-7,8,9,10-  
tetrahydro-10-oxo-6-[6-(trimethylsilyl)-3-hexene-1,5-diy-nyl]-, phenyl  
ester, [6 $\alpha$ (Z),6 $\alpha$  $\beta$ ,10 $\alpha$  $\beta$ ]- (9CI) (CA INDEX NAME)

Relative stereochemistry.

Double bond geometry as shown.



OS.CITING REF COUNT: 7 THERE ARE 7 CAPLUS RECORDS THAT CITE THIS RECORD  
(7 CITINGS)

L8 ANSWER 37 OF 39 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1992:633659 CAPLUS [Full-text](#)

DOCUMENT NUMBER: 117:233659

ORIGINAL REFERENCE NO.: 117:40395a,40398a

TITLE: Molecular design and chemical synthesis of potent  
enediynes. 1. Dymenicin model systems equipped with  
N-tethered triggering devices

AUTHOR(S): Nicolaou, K. C.; Maligres, P.; Suzuki, T.; Wendeborn,  
S. V.; Dai, W. M.; Chadha, R. K.

CORPORATE SOURCE: Dep. Chem., Scripps Res. Inst., La Jolla, CA, 92037,  
USA

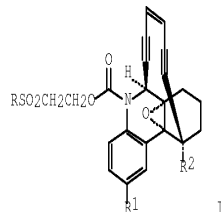
SOURCE: Journal of the American Chemical Society (1992),  
114(23), 8890-907

CODEN: JACSAT; ISSN: 0002-7863

DOCUMENT TYPE: Journal

LANGUAGE: English

GI



AB In this article the mol. design and chemical synthesis of a series of  
enediynes I (R = Ph, 1-naphthyl, 2-naphthyl; R1 = H, MeO, HOCH2CH2O,  
HOCH2C.tpbond.C; R2 = H, MeO, HOCH2CH2O) related to the dymenicin A structure  
and carrying N-tethered triggering devices are described. The design  
envisioned the [(arylsulfonyl)ethoxy]carbonyl group attached at the nitrogen  
atom as a triggering device for the Bergman cycloaromatization reaction  
because of its ability to undergo  $\beta$ -elimination under basic conditions,  
liberating the labile free amine intermediate. A number of tethering groups  
on the aromatic ring were also installed in these systems for future  
incorporation of other desirable moieties such as delivery systems and  
solubility enhancers. Bergman cycloaromatization expts. under basic and  
acidic conditions demonstrated the abilities of these compds. to generate  
benzenoid diradicals. A number of potent DNA-cleaving compds. and cytotoxic  
agents emerged from these studies.

IT 144127-80-0F

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT  
(Reactant or reagent)

(preparation and desilylation of)

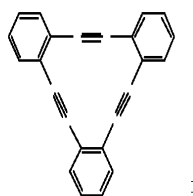
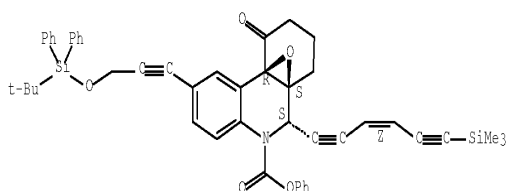
RN 144127-80-0 CAPLUS

CN 6a,10a-Epoxyphenanthridine-5(6H)-carboxylic acid,  
2-[3-[[[1,1-dimethylethyl]diphenylsilyl]oxy]-1-propynyl]-7,8,9,10-  
tetrahydro-10-oxo-6-[6-(trimethylsilyl)-3-hexene-1,5-diy-nyl]-, phenyl  
ester, [6 $\alpha$ (Z),6 $\alpha$  $\beta$ ,10 $\alpha$  $\beta$ ]- (9CI) (CA INDEX NAME)

Relative stereochemistry.

Double bond geometry as shown.





I

IT 144127-81-1P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

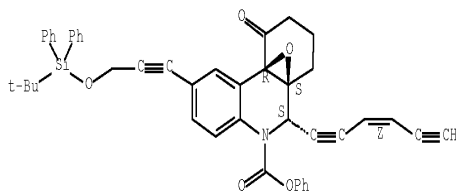
(preparation and intramol. cycloaddn. reaction of, epoxyhexenediynophenanthridine from)

RN 144127-81-1 CAPLUS

CN 6a,10a-Epoxyphenanthridine-5(6H)-carboxylic acid, 2-[3-[[[1,1-dimethylethyl)diphenylsilyl]oxy]-1-propynyl]-6-(3-hexene-1,5-diynyl)-7,8,9,10-tetrahydro-10-oxo-, phenyl ester, [6 $\alpha$ (Z),6 $\alpha$  $\beta$ ,10 $\alpha$  $\beta$ ]- (9CI) (CA INDEX NAME)

Relative stereochemistry.

Double bond geometry as shown.



AB A novel synthesis of dehydro[12]annulenes from o-Br2C6H4 is based on selective Pd(0)-Cu(I) coupling reactions of aryl and vinyl halides with terminal acetylenes. Thus, coupling reaction of o-Br2C6H4 with HC.tplbond.CCMe2OH gave 63% o-BrC6H4C.tplbond.CCMe2OH. Cleavage with NaOH followed by in situ trimerization gave 36% dehydroannulene I.

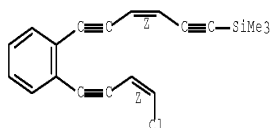
IT 120651-32-3P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(preparation and desilylation of)

RN 120651-32-3 CAPLUS

CN Silane, [6-[2-(4-chloro-3-buten-1-ynyl)phenyl]-3-hexene-1,5-diynyl]trimethyl-, (Z,Z)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



OS.CITING REF COUNT: 31 THERE ARE 31 CAPLUS RECORDS THAT CITE THIS RECORD (31 CITINGS)

L8 ANSWER 38 OF 39 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1989:212183 CAPLUS [Full-text](#)

DOCUMENT NUMBER: 110:212183

ORIGINAL REFERENCE NO.: 110:35199a,35202a

TITLE: A short route to dehydro[12]annulenes

AUTHOR(S): Huynh Chanh; Linstrumelle, Gerard

CORPORATE SOURCE: Lab. Chim., Ec. Norm. Super., Paris, 75231, Fr.

SOURCE: Tetrahedron (1988), 44(20), 6337-44

CODEN: TETRAB; ISSN: 0040-4020

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 110:212183

GI

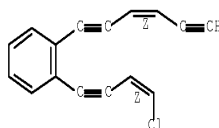
IT 120651-36-7P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(preparation and intramol. coupling reaction of, dehydroannulene from)

RN 120651-36-7 CAPLUS

CN Benzene, 1-(4-chloro-3-buten-1-ynyl)-2-(3-hexene-1,5-diynyl)-, (Z,Z)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



L8 ANSWER 39 OF 39 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1968:78330 CAPLUS [Full-text](#)

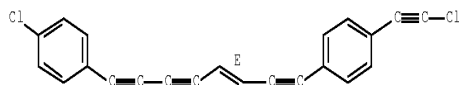


DOCUMENT NUMBER: 68:78330  
 ORIGINAL REFERENCE NO.: 68:15123a,15126a  
 TITLE: Interaction of diiodoethylene with copper acetylides  
 AUTHOR(S): Ukhin, L. Yu.; Sladkov, A. M.; Gorshkov, V. I.  
 CORPORATE SOURCE: Inst. Elementoorg. Soedin, Moscow, USSR  
 SOURCE: Zhurnal Organicheskoi Khimii (1968), 4(1), 25-7  
 CODEN: ZORKAE; ISSN: 0514-7492  
 DOCUMENT TYPE: Journal  
 LANGUAGE: Russian

AB Reaction of trans-diiodoethylene (I) with Cu acetylides gave the condensation products of general formula RC.tplbond.CCH:CHI (IIa) or RC.tplbond.CCH:CHC.tplbond.CR (IIb). The structure of products was confirmed by ir and mass spectroscopy; trans configuration of the double bond was preserved. For example, a mixture of 3.29 g. (PhC.tplbond.C)2Cu, 2.78 g. I, and 100 ml. HCONMe2 was stirred 4 hrs. at 90° and then refluxed 2 hrs. Cooling, filtration, and addition of H2O to the filtrate precipitated 56% IIb (R = Ph) m. 111-12° (heptane). Similarly, IIb (R = Bu) b4 117°, n24D 1.5173 was prepared Boiling 23.4 g. (BuC.tplbond.C)2Cu with 44.8 g. I in 125 ml. pyridine for 10 min. gave 40% IIa (R = Bu) b5 84-5°, n20D 1.5519. Similarly IIa (R = Ph) b2.5 112-14°, n23D 1.6880 was prepared However boiling (p-IC6H4C.tplbond.C)2Cu, with I in pyridine gave IIa (R = p-IC6H4) m. 125-30° and IIb (R = p-IC6H4) m. 245-7° (C6H6-heptane), separated by crystallization Also (p-ClC6H4C.tplbond.C)2Cu and I gave IIa (R = p-ClC6H4C.tplbond.C) m. 80-5° and IIb (R = p-ClC6H4C.tplbond.C) m. 179-85° (heptane). To further confirm the structures of IIa and IIb they were converted to boranes by refluxing with an excess of decaborane in PhMe solution The following were characterized (compound, % yield, and m.p. given): 1,2-bis(1-butylbarenyl)ethylene, 62, 153-5° (PhMe); 1-(β-iodovinyl)-2-phenylbarene, -, 227-35° (hexane); 1-(β-iodovinyl)-2-butylbarene, -, 72-4°.

IT 1582669-94-0F  
 RL: SPN (Synthetic preparation); PRP (Properties); PREP (Preparation)  
 (Interaction of diiodoethylene with copper acetylides)  
 RN 1082669-94-0 CAPLUS  
 CN INDEX NAME NOT YET ASSIGNED

Double bond geometry as shown.



FILE 'HOME' ENTERED AT 10:26:39 ON 18 DEC 2009

=> file registry

=>  
 Uploading C:\Program Files\STNEXP\Queries\10591950-claim 1-v 3.str



chain nodes :  
 1 2 3 4 5 6 7 8 9 11 12  
 chain bonds :  
 1-2 1-12 2-3 3-4 4-5 5-6 6-7 7-8 8-9 9-11  
 exact/norm bonds :  
 6-7 7-8  
 exact bonds :  
 1-2 1-12 2-3 3-4 4-5 5-6 8-9 9-11

G1:Cb,Cy,Hy

Match level :  
 1:CLASS 2:CLASS 3:CLASS 4:CLASS 5:CLASS 6:CLASS 7:CLASS 8:CLASS 9:CLASS  
 11:CLASS 12:CLASS

L1 STRUCTURE UPLOADED

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 SAMPLE SCREEN SEARCH COMPLETED - 72 TO ITERATE

100.0% PROCESSED 72 ITERATIONS 1 ANSWERS  
 SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*  
 BATCH \*\*COMPLETE\*\*  
 PROJECTED ITERATIONS: 931 TO 1949  
 PROJECTED ANSWERS: 1 TO 80

L2 1 SEA SSS SAM L1

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 SEARCH TIME: 00.00.01

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=> s l3



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YOU HAVE REQUESTED DATA FROM 11 ANSWERS - CONTINUE? Y/(N):y

L4 ANSWER 1 OF 11 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 2009:1167687 CAPLUS [Full-text](#)

DOCUMENT NUMBER: 151:470282

TITLE: Synthesis of hybrid masked triyne-phenylene axial rods containing (E)- $\beta$ -chlorovinylsilanes in the  $\pi$ -conjugated framework

AUTHOR(S): Weller, Michael D.; Kariuki, Benson M.; Cox, Liam R.

CORPORATE SOURCE: School of Chemistry, The University of Birmingham, Birmingham, B15 2TT, UK

SOURCE: Journal of Organic Chemistry (2009), 74(20), 7898-7907  
CODEN: JOCEAH; ISSN: 0022-3263

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Silyl-masked hexayne Me<sub>3</sub>SiC.tplbond.CCCl:C(SiR<sub>3</sub>)C.tplbond.CC.tplbond.C(SiR<sub>3</sub>):CClC.tplbond.CSiMe<sub>3</sub> (7, SiR<sub>3</sub> = tBuPh<sub>2</sub>Si) undergoes fluoride-induced  $\beta$ -elimination yielding, after terminal modifications, 1,12-diaryldodecahexaynes; compared to its positional isomer

Me<sub>3</sub>SiC.tplbond.CC(SiR<sub>3</sub>):CClC.tplbond.CC.tplbond.CCl:C(SiR<sub>3</sub>)C.tplbond.CSiMe<sub>3</sub> (2, same SiR<sub>3</sub>), prepared earlier, the compound 7 provides increased flexibility, allowing introduction of aromatic spacer groups, useful in production of carbyne-type mol. wires. A two-directional synthesis of a masked hexayne 7, in which two  $\beta$ -chlorovinylsilanes protect two of the internal alkynes, is reported. The key step involves the Pd-catalyzed oxidative dimerization of alkyne HC.tplbond.CC(SiR<sub>3</sub>):CClCH<sub>2</sub>OTHP (10) to provide diyne THPOCH<sub>2</sub>CCl:C(SiR<sub>3</sub>)C.tplbond.CC.tplbond.CC(SiR<sub>3</sub>):CClCH<sub>2</sub>OTHP (12), which is elaborated into centrosym. masked hexayne 7 in four steps. Masked hexayne 7 is a constitutional isomer of masked hexayne 2, which has been used as a monomer unit for oligoyne assembly. Although masked hexayne 7 was not as convenient a building block as 2 for application in oligoyne assembly, one of its precursors, namely alkyne 10, could be used successfully in Sonogashira couplings, which allowed the incorporation of aromatic spacers and the formation of hybrid masked triyne-phenylenes

Me<sub>3</sub>SiC.tplbond.CCCl:C(SiR<sub>3</sub>)C.tplbond.C-1,4-C<sub>6</sub>H<sub>4</sub>C.tplbond.CC(SiR<sub>3</sub>):CClC.tplbond.CSiMe<sub>3</sub> (20) and [Me<sub>3</sub>SiC.tplbond.CCCl:C(SiR<sub>3</sub>)C.tplbond.C-1,4-C<sub>6</sub>H<sub>4</sub>C.tplbond.C]2 (28). Comps. 20 and 28 both contain removable end-groups, which will permit their application as building blocks for the assembly of classes of long-chain,  $\pi$ -conjugated rod-like mols. Rod-like mol.

Me<sub>2</sub>C(OH)C.tplbond.CCCl:C(SiR<sub>3</sub>)C.tplbond.CC<sub>6</sub>H<sub>4</sub>C.tplbond.C]2C(SiR<sub>3</sub>):CClC.tplbond.CCMe<sub>2</sub>(OH) (34, C<sub>6</sub>H<sub>4</sub> = 1,4-phenylene), which possesses a similar conjugated scaffold as 28, was also prepared by using a similar strategy. Treatment of 34 with TBAF effected a 2-fold dechlorosilylation to provide a rigid rod mol. Me<sub>2</sub>C(OH)C.tplbond.C]3C<sub>6</sub>H<sub>4</sub>C.tplbond.C]2C<sub>6</sub>H<sub>4</sub>C.tplbond.C]3CMe<sub>2</sub>(OH) (35) in which two 1,4-phenylene units interrupt an octayne scaffold.

IT 1191093-35-2P 1191093-44-3P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

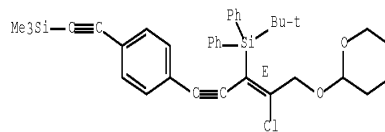
(preparation of  $\pi$ -conjugated p-phenylene-bridged  $\beta$ -chloro silyl-substituted enynes as precursors for arylene-containing polyyne mol. wires)

RN 1191093-35-2 CAPLUS

CN 2H-Pyran, 2-[[[(2E)-2-chloro-3-[(1,1-dimethylethyl)diphenylsilyl]-5-[4-[2-(trimethylsilyl)ethynyl]phenyl]-2-penten-4-yn-1-yl]oxy]tetrahydro- (CA

INDEX NAME)

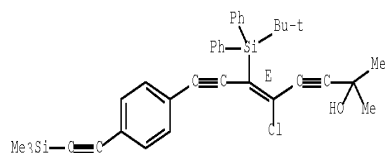
Double bond geometry as shown.



RN 1191093-44-3 CAPLUS

CN INDEX NAME NOT YET ASSIGNED

Double bond geometry as shown.



REFERENCE COUNT: 60 THERE ARE 60 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 2 OF 11 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 2005:1004691 CAPLUS [Full-text](#)

DOCUMENT NUMBER: 143:306181

TITLE: Process for preparation of  $\pi$ -conjugated aromatic ring-containing acetylene derivatives as organic electroluminescent devices

INVENTOR(S): Sato, Fumie; Takayama, Yuuki

PATENT ASSIGNEE(S): Nissan Chemical Industries, Ltd., Japan

SOURCE: PCT Int. Appl., 82 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: Japanese

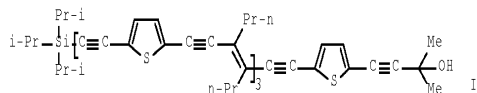
FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005085176	A1	20050915	WO 2005-JP3950	20050308
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, GR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MY, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML,				



MR, NE, SN, TD, TG  
 US 20070176164 A1 20070802 US 2007-591950 20070307  
 PRIORITY APPLN. INFO.: JP 2004-65446 A 20040309  
 WO 2005-JP3950 W 20050308  
 ASSIGNMENT HISTORY FOR US PATENT AVAILABLE IN LSUS DISPLAY FORMAT  
 OTHER SOURCE(S): MARPAT 143:306181  
 GI



AB This invention pertains to a method for producing  $\pi$ -conjugated aromatic ring-containing acetylene derivs. via coupling reaction in the presence of palladium and Cu(I) catalysts. For example, the compound I was prepared in a multi-step synthesis in good yield. The title compds. are useful as electroluminescent devices.

IT 740810-59-7P 740810-60-0P 740810-61-4P  
 740810-65-5P 740810-67-7P 740810-68-8P  
 864683-35-4P 864684-00-4P 864684-04-4P  
 864684-05-3P 864684-31-1P

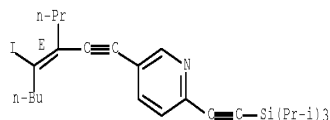
RL: IMF (Industrial manufacture); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(intermediate; preparation of  $\pi$ -conjugated aromatic ring-containing acetylene derivs. as organic electroluminescent devices)

RN 740810-59-7 CAPLUS

CN Pyridine, 5-[(3E)-4-iodo-3-propyl-3-octen-1-yn-1-yl]-2-[2-[tris(1-methylethyl)silyl]ethynyl]- (CA INDEX NAME)

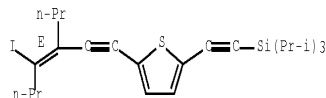
Double bond geometry as shown.



RN 740810-60-0 CAPLUS

CN Thiophene, 2-[(3E)-4-iodo-3-propyl-3-hepten-1-yn-1-yl]-5-[2-[tris(1-methylethyl)silyl]ethynyl]- (CA INDEX NAME)

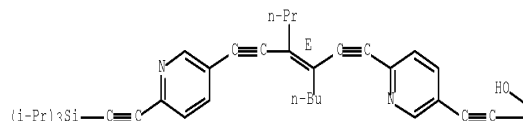
Double bond geometry as shown.



RN 740810-64-4 CAPLUS

CN 3-Butyn-2-ol, 4-[6-[(3E)-3-butyl-4-[2-[6-[2-[tris(1-methylethyl)silyl]ethynyl]-3-pyridinyl]ethynyl]-3-hepten-1-yn-1-yl]-3-pyridinyl]-2-methyl- (CA INDEX NAME)

Double bond geometry as shown.



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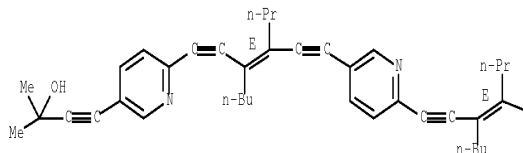


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RN 740810-65-5 CAPLUS

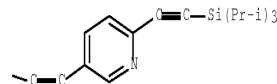
CN 3-Butyn-2-ol, 4-[6-[(3E)-3-butyl-4-[2-[6-[(3E)-3-butyl-4-[2-[6-[2-[tris(1-methylethyl)silyl]ethynyl]-3-pyridinyl]ethynyl]-3-hepten-1-yn-1-yl]-3-pyridinyl]ethynyl]-3-hepten-1-yn-1-yl]-3-pyridinyl]-2-methyl- (CA INDEX NAME)

Double bond geometry as shown.



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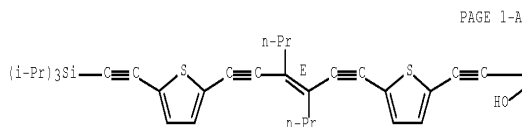
PAGE 1-B





RN 740810-67-7 CAPLUS  
 CN 3-Butyn-2-ol, 2-methyl-4-[5-[(3E)-3-propyl-4-[[5-[[tris(1-methylethyl)silyl]ethynyl]-2-thienyl]ethynyl]-3-hepten-1-yn-1-yl]-2-thienyl]- (CA INDEX NAME)

Double bond geometry as shown.

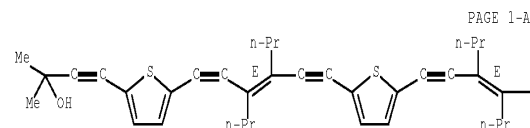


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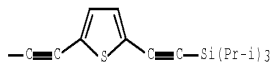


RN 740810-68-8 CAPLUS  
 CN 3-Butyn-2-ol, 2-methyl-4-[5-[(3E)-3-propyl-4-[[5-[(3E)-3-propyl-4-[[5-[[tris(1-methylethyl)silyl]ethynyl]-2-thienyl]ethynyl]-3-hepten-1-yn-1-yl]-2-thienyl]ethynyl]-3-hepten-1-yn-1-yl]-2-thienyl]- (CA INDEX NAME)

Double bond geometry as shown.

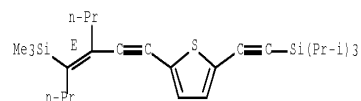


PAGE 1-B



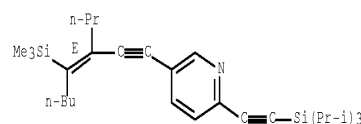
RN 864683-95-4 CAPLUS  
 CN Thiophene, 2-[(3E)-3-propyl-4-(trimethylsilyl)-3-hepten-1-yn-1-yl]-5-[2-[tris(1-methylethyl)silyl]ethynyl]- (CA INDEX NAME)

Double bond geometry as shown.



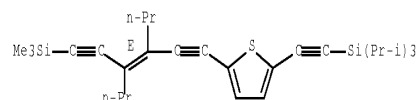
RN 864684-00-4 CAPLUS  
 CN Pyridine, 5-[(3E)-3-propyl-4-(trimethylsilyl)-3-octen-1-yn-1-yl]-2-[2-[tris(1-methylethyl)silyl]ethynyl]- (CA INDEX NAME)

Double bond geometry as shown.



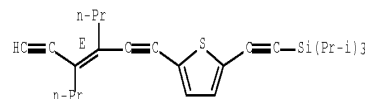
RN 864684-04-8 CAPLUS  
 CN Thiophene, 2-[(3E)-3,4-dipropyl-6-(trimethylsilyl)-3-hexene-1,5-diyn-1-yl]-5-[2-[tris(1-methylethyl)silyl]ethynyl]- (CA INDEX NAME)

Double bond geometry as shown.



RN 864684-05-9 CAPLUS  
 CN Thiophene, 2-[(3E)-4-ethynyl-3-propyl-3-hepten-1-yn-1-yl]-5-[2-[tris(1-methylethyl)silyl]ethynyl]- (CA INDEX NAME)

Double bond geometry as shown.



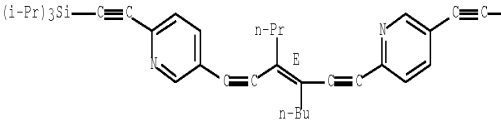
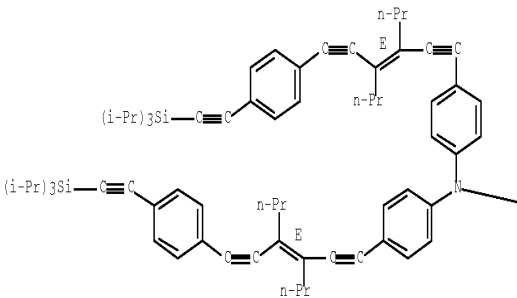
RN 864684-31-1 CAPLUS  
 CN Benzenamine, N-[4-[(3E)-3,4-dipropyl-6-[4-[2-[tris(1-methylethyl)silyl]ethynyl]phenyl]-3-hexene-1,5-diyn-1-yl]phenyl]-4-[(3E)-3-propyl-4-[2-[4-[2-[tris(1-methylethyl)silyl]ethynyl]phenyl]ethynyl]-3-hepten-1-yn-1-yl]-N-[4-[(3E)-3-propyl-4-[2-[4-[2-[tris(1-methylethyl)silyl]ethynyl]phenyl]ethynyl]-3-hepten-1-yn-1-yl]phenyl]- (CA INDEX NAME)



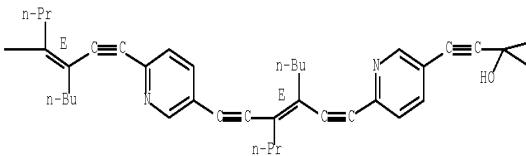
Double bond geometry as shown.

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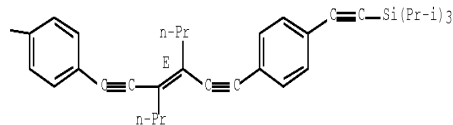
PAGE 1-A



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PAGE 1-C

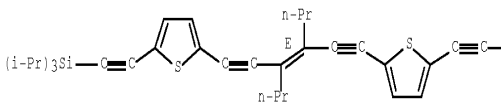


IT 740810-66-6P 740810-68-8P 864684-06-0P  
864684-21-3P 864684-22-0P 864684-23-1P  
864684-24-2P 864684-25-3P 864684-26-4P  
864684-27-5P 864684-28-6P 864684-29-7P  
864684-30-8P  
RL: DEV (Device component use); IMF (Industrial manufacture); SPN  
(Synthetic preparation); TEM (Technical or engineered material use); PREP  
(Preparation); USES (Uses)  
(preparation of  $\pi$ -conjugated aromatic ring-containing acetylene derivs. as  
organic electroluminescent devices)

RN 740810-66-6 CAPLUS  
CN 3-Butyn-2-ol, 4-[6-[(3E)-3-butyl-4-[2-[6-[(3E)-3-butyl-4-[2-[6-[(3E)-3-  
butyl-4-[2-[6-[2-[tris(1-methylethyl)silyl]ethynyl]-3-pyridinyl]ethynyl]-3-  
hepten-1-yn-1-yl]-3-pyridinyl]ethynyl]-3-hepten-1-yn-1-yl]-3-  
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NAME)

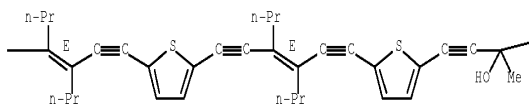
Double bond geometry as shown.

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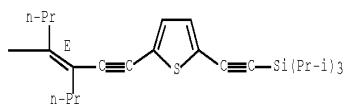




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RN 864684-22-0 CAPLUS

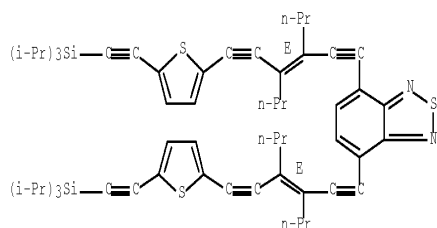
CN Benzene, 1-[(3E)-3,4-dipropyl-6-[4-[2-[tris(1-methylethyl)silyl]ethynyl]phenyl]-3-hexene-1,5-diyn-1-yl]-4-[(3E)-3-propyl-4-[2-[4-[2-[tris(1-methylethyl)silyl]ethynyl]phenyl]ethynyl]-3-hepten-1-yn-1-yl]- (CA INDEX NAME)

Double bond geometry as shown.

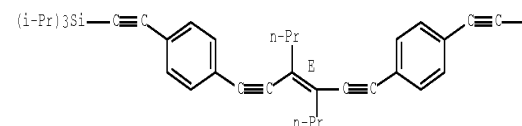
RN 864684-06-0 CAPLUS

CN 2,1,3-Benzothiadiazole, 4-[(3E)-3,4-dipropyl-6-[5-[2-[tris(1-methylethyl)silyl]ethynyl]-2-thienyl]-3-hexene-1,5-diyn-1-yl]-7-[(3E)-3-propyl-4-[2-[5-[2-[tris(1-methylethyl)silyl]ethynyl]-2-thienyl]ethynyl]-3-hepten-1-yn-1-yl]- (CA INDEX NAME)

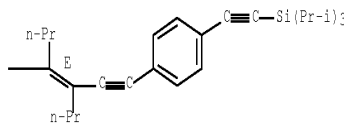
Double bond geometry as shown.



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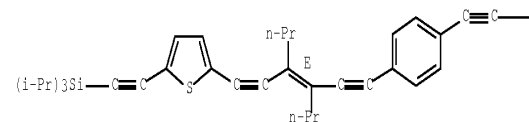


RN 864684-21-9 CAPLUS

CN Thiophene, 2-[(3E)-3,4-dipropyl-6-[4-[(3E)-3-propyl-4-[2-[5-[2-[tris(1-methylethyl)silyl]ethynyl]-2-thienyl]ethynyl]-3-hepten-1-yn-1-yl]phenyl]-3-hexene-1,5-diyn-1-yl]-5-[2-[tris(1-methylethyl)silyl]ethynyl]- (CA INDEX NAME)

Double bond geometry as shown.

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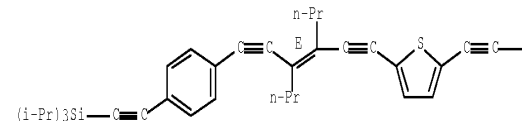


RN 864684-23-1 CAPLUS

CN Thiophene, 2-[(3E)-3,4-dipropyl-6-[4-[2-[tris(1-methylethyl)silyl]ethynyl]phenyl]-3-hexene-1,5-diyn-1-yl]-5-[(3E)-3-propyl-4-[2-[4-[2-[tris(1-methylethyl)silyl]ethynyl]phenyl]ethynyl]-3-hepten-1-yn-1-yl]- (CA INDEX NAME)

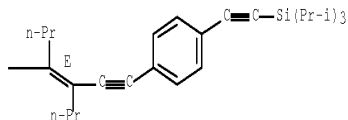
Double bond geometry as shown.

PAGE 1-A





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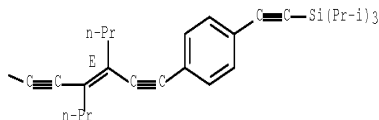


RN 864684-24-2 CAPLUS

CN Silane, [oxybis[4,1-phenylene[(3E)-3,4-dipropyl-3-hexene-1,5-diyne-6,1-diyl]-4,1-phenylene-2,1-ethynediyl]]bis[tris(1-methylethyl)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

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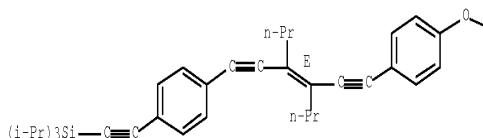


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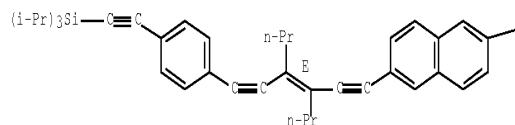
CN Naphthalene, 2-[(3E)-3,4-dipropyl-6-[4-[2-[tris(1-methylethyl)silyl]ethynyl]phenyl]-3-hexene-1,5-diyn-1-yl]-6-[(3E)-3-propyl-4-[2-[4-[2-[tris(1-methylethyl)silyl]ethynyl]phenyl]ethynyl]-3-hepten-1-yn-1-yl]- (CA INDEX NAME)

Double bond geometry as shown.

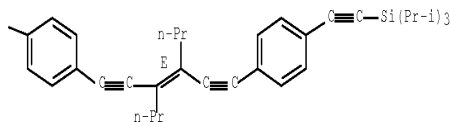
PAGE 1-A



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PAGE 1-B

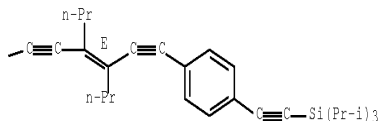


RN 864684-25-3 CAPLUS

CN 2,2'-Bithiophene, 5-[(3E)-3,4-dipropyl-6-[4-[2-[tris(1-methylethyl)silyl]ethynyl]phenyl]-3-hexene-1,5-diyn-1-yl]-5'-[(3E)-3-propyl-4-[2-[4-[2-[tris(1-methylethyl)silyl]ethynyl]phenyl]ethynyl]-3-hepten-1-yn-1-yl]- (CA INDEX NAME)

Double bond geometry as shown.

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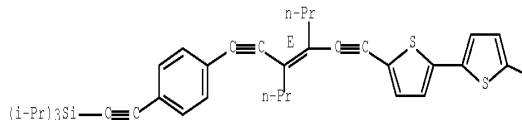


RN 864684-27-5 CAPLUS

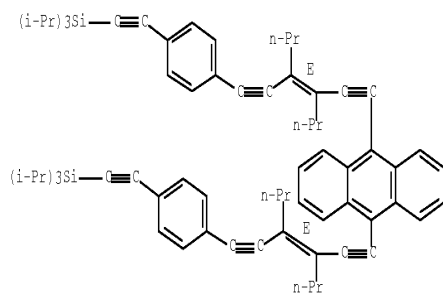
CN Anthracene, 9-[(3E)-3,4-dipropyl-6-[4-[2-[tris(1-methylethyl)silyl]ethynyl]phenyl]-3-hexene-1,5-diyn-1-yl]-10-[(3E)-3-propyl-4-[2-[4-[2-[tris(1-methylethyl)silyl]ethynyl]phenyl]ethynyl]-3-hepten-1-yn-1-yl]- (CA INDEX NAME)

Double bond geometry as shown.

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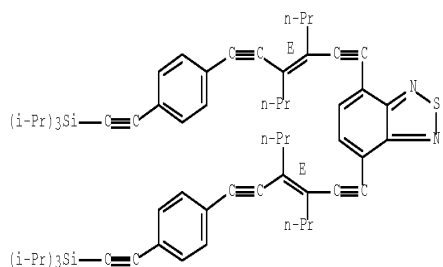




RN 864684-28-6 CAPLUS

CN 2,1,3-Benzothiadiazole, 4-[(3E)-3,4-dipropyl-6-[4-[2-[tris(1-methylethyl)silyl]ethynyl]phenyl]-3-hexene-1,5-diyn-1-yl]-7-[(3E)-3-propyl-4-[2-[4-[2-[tris(1-methylethyl)silyl]ethynyl]phenyl]ethynyl]-3-hepten-1-yn-1-yl]- (CA INDEX NAME)

Double bond geometry as shown.

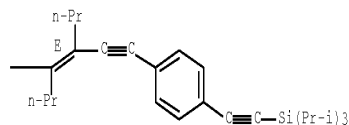
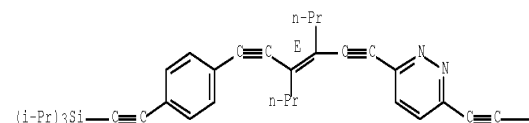


RN 864684-29-7 CAPLUS

CN Pyridazine, 3-[(3E)-3,4-dipropyl-6-[4-[2-[tris(1-methylethyl)silyl]ethynyl]phenyl]-3-hexene-1,5-diyn-1-yl]-6-[(3E)-3-propyl-4-[2-[4-[2-[tris(1-methylethyl)silyl]ethynyl]phenyl]ethynyl]-3-hepten-1-yn-1-yl]- (CA INDEX NAME)

Double bond geometry as shown.

PAGE 1-A

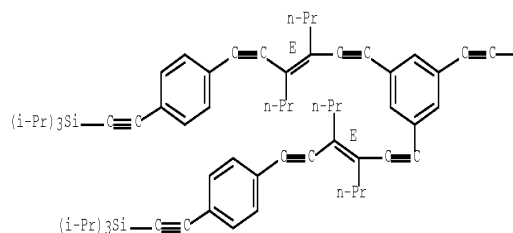


RN 864684-30-0 CAPLUS

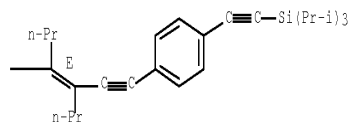
CN Benzene, 1-[(3E)-3,4-dipropyl-6-[4-[2-[tris(1-methylethyl)silyl]ethynyl]phenyl]-3-hexene-1,5-diyn-1-yl]-3-[(3E)-5-ethyl-3-propyl-4-[2-[4-[2-[tris(1-methylethyl)silyl]ethynyl]phenyl]ethynyl]-3-penten-1-yn-1-yl]-5-[(3E)-3-propyl-4-[2-[4-[2-[tris(1-methylethyl)silyl]ethynyl]phenyl]ethynyl]-3-hepten-1-yn-1-yl]- (CA INDEX NAME)

Double bond geometry as shown.

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PAGE 1-B



IT 740810-57-5

RL: RCT (Reactant); RACT (Reactant or reagent)

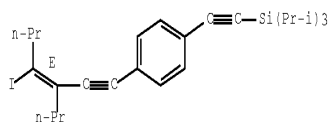
(preparation of  $\pi$ -conjugated aromatic ring-containing acetylene derivs. as organic electroluminescent devices)

RN 740810-57-5 CAPLUS

CN Benzene, 1-[(3E)-4-iodo-3-propyl-3-hepten-1-yn-1-yl]-4-[2-[tris(1-methylethyl)silyl]ethynyl]- (CA INDEX NAME)

Double bond geometry as shown.



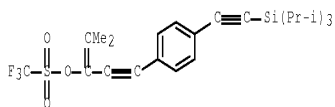


REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 3 OF 11 CAPLUS COPYRIGHT 2009 ACS on STN  
 ACCESSION NUMBER: 2005:509432 CAPLUS [Full-text](#)  
 DOCUMENT NUMBER: 143:7446  
 TITLE: Synthesis and characterization of cross-conjugated oligo(phenylene enynylene)s  
 AUTHOR(S): Cho, Joon; Zhao, Yuming; Tykwinski, Rik R.  
 CORPORATE SOURCE: Department of Chemistry, University of Alberta, Edmonton, AB, T6G 2G2, Can.  
 SOURCE: ARKIVOC (Gainesville, FL, United States) (2005), (4), 142-150  
 CODEN: AGFUAR  
 URL: [http://www.arkat-usa.org/ark/journal/2005/I04\\_Zefirov/1369/1369.pdf](http://www.arkat-usa.org/ark/journal/2005/I04_Zefirov/1369/1369.pdf)  
 PUBLISHER: Arkat USA Inc.  
 DOCUMENT TYPE: Journal; (online computer file)  
 LANGUAGE: English  
 OTHER SOURCE(S): CASREACT 143:7446

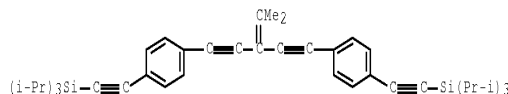
AB The synthesis and characterization of a series of cross-conjugated oligo(phenylene enynylene)s via the Sonogashira protocol is reported. The structural properties of these oligomers have been established by <sup>1</sup>H and <sup>13</sup>C NMR and IR spectroscopies, as well as mass spectrometry. Their electronic absorption and emission behavior has been investigated via UV/Vis and fluorescence spectroscopy. The results of this study demonstrate that electronic communication along the conjugated framework of these oligomers is limited due to the presence of a cross-conjugated enyne framework and arylene fragments.

IT 852459-83-7P 852459-85-3P  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
 (preparation of cross-conjugated oligo(phenylene enynylene)s via the Sonogashira reaction)  
 RN 852459-83-7 CAPLUS  
 CN Methanesulfonic acid, 1,1,1-trifluoro-, 2-methyl-1-[2-[4-[2-[tris(1-methylethyl)silyl]ethynyl]phenyl]ethynyl]-1-propen-1-yl ester (CA INDEX NAME)

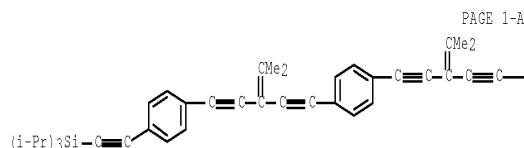


RN 852459-85-9 CAPLUS

CN Benzene, 1-[4-methyl-3-[2-[4-[2-[tris(1-methylethyl)silyl]ethynyl]phenyl]ethynyl]-3-penten-1-yn-1-yl]-4-[2-[tris(1-methylethyl)silyl]ethynyl]- (CA INDEX NAME)

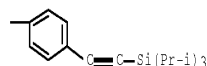


IT 852459-83-7P 852459-85-3P  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (preparation of cross-conjugated oligo(phenylene enynylene)s via the Sonogashira reaction)  
 RN 852459-86-0 CAPLUS  
 CN Benzene, 1,4-bis[4-methyl-3-[2-[4-[2-[tris(1-methylethyl)silyl]ethynyl]phenyl]ethynyl]-3-penten-1-yn-1-yl]- (CA INDEX NAME)

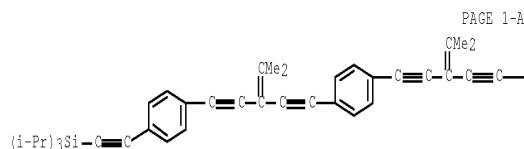


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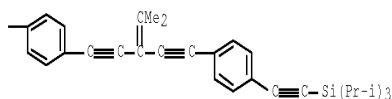
RN 852459-87-1 CAPLUS  
 CN Benzene, 1-[4-methyl-3-[2-[4-[4-methyl-3-[2-[4-[2-[tris(1-methylethyl)silyl]ethynyl]phenyl]ethynyl]-3-penten-1-yn-1-yl]phenyl]ethynyl]-3-penten-1-yn-1-yl]-4-[4-methyl-3-[2-[4-[2-[tris(1-methylethyl)silyl]ethynyl]phenyl]ethynyl]-3-penten-1-yn-1-yl]- (CA INDEX NAME)



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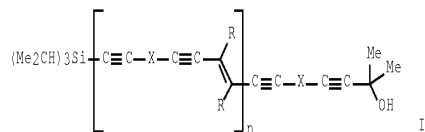


PAGE 1-B



REFERENCE COUNT: 20 THERE ARE 20 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

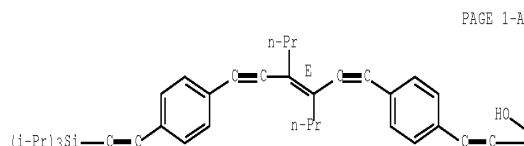
L4 ANSWER 4 OF 11 CAPLUS COPYRIGHT 2009 ACS on STN  
 ACCESSION NUMBER: 2004:480115 CAPLUS Full-text  
 DOCUMENT NUMBER: 141:190674  
 TITLE: Synthesis of Conjugated Oligomers Having Aromatic and Enediyne Units Alternately in the Backbone that Show Intense Fluorescence Emission  
 AUTHOR(S): Nakano, Yuuki; Ishizuka, Kenichi; Muraoka, Kenji; Ohtani, Hiroyuki; Takayama, Yuuki; Sato, Fumie  
 CORPORATE SOURCE: Department of Biomolecular Engineering, Tokyo Institute of Technology, Midori, Yokohama, Kanagawa, 226-8501, Japan  
 SOURCE: Organic Letters (2004), 6(14), 2373-2376  
 CODEN: ORLEF7; ISSN: 1523-7060  
 PUBLISHER: American Chemical Society  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 OTHER SOURCE(S): CASREACT 141:190674  
 GI



AB Synthesis and fluorescence properties of  $\pi$ -conjugated compds. I (n = 1 - 3; X = 1,4-phenylene, 2,5-pyridine, 2,5-thiophene; R = n-Pr, n-Bu) having alternately an aromatic or heteroarom. ring and an enediyne unit in the backbone are described.  
 IT 740810-61-1P 740810-62-2P 740810-64-4P  
 740810-65-5P 740810-67-7P 740810-68-8P  
 RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
 (preparation and absorption and fluorescence spectra of conjugated oligomers having aromatic (or heteroarom.) and enediyne units alternately in the

backbone)  
 RN 740810-61-1 CAPLUS  
 CN 3-Butyn-2-ol, 2-methyl-4-[4-[(3E)-3-propyl-4-[2-[4-[2-[tris(1-methylethyl)silyl]ethynyl]phenyl]ethynyl]-3-hepten-1-yn-1-yl]phenyl]- (CA INDEX NAME)

Double bond geometry as shown.



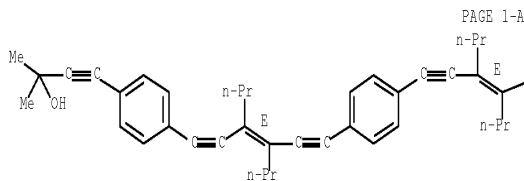
PAGE 1-A

PAGE 1-B



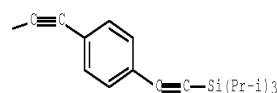
RN 740810-62-2 CAPLUS  
 CN 3-Butyn-2-ol, 2-methyl-4-[4-[(3E)-3-propyl-4-[[4-[(3E)-3-propyl-4-[[4-[[tris(1-methylethyl)silyl]ethynyl]phenyl]ethynyl]-3-hepten-1-yn-1-yl]phenyl]ethynyl]-3-hepten-1-yn-1-yl]phenyl]- (CA INDEX NAME)

Double bond geometry as shown.



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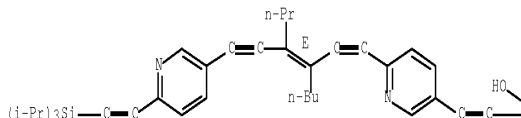
PAGE 1-B





CN 3-Butyn-2-ol, 4-[6-[(3E)-3-butyl-4-[2-[6-[2-[tris(1-methylethyl)silyl]ethynyl]-3-pyridinyl]ethynyl]-3-hepten-1-yn-1-yl]-3-pyridinyl]-2-methyl- (CA INDEX NAME)

PAGE 1-A

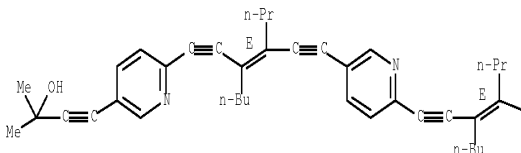


PAGE 1-B

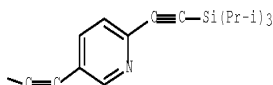


CN 3-Butyn-2-ol, 4-[6-[(3E)-3-butyl-4-[2-[6-[(3E)-3-butyl-4-[2-[6-[2-[tris(1-methylethyl)silyl]ethynyl]-3-pyridinyl]ethynyl]-3-hepten-1-yn-1-yl]-3-pyridinyl]ethynyl]-3-hepten-1-yn-1-yl]-3-pyridinyl]-2-methyl- (CA INDEX NAME)

PAGE 1-A

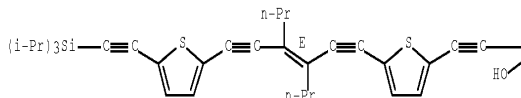


PAGE 1-B



CN 3-Butyn-2-ol, 2-methyl-4-[5-[ (3E)-3-propyl-4-[ [5-[ (tris(1-methylethyl)silyl)ethynyl]-2-thienyl)ethynyl]-3-hepten-1-yn-1-yl]-2-thienyl]- (CA INDEX NAME)

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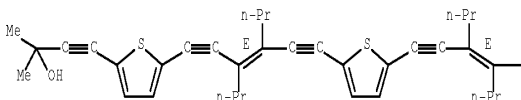


PAGE 1-B

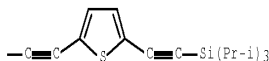


CN 3-Butyn-2-ol, 2-methyl-4-[5-[(3E)-3-propyl-4-[[5-[(3E)-3-propyl-4-[[5-  
[[tris(1-methylethyl)silyl]ethynyl]-2-thienyl]ethynyl]-3-hepten-1-yn-1-yl]-  
2-thienyl]ethynyl]-3-hepten-1-yn-1-yl]-2-thienyl)- (CA INDEX NAME)

PAGE 1-A



PAGE 1-B



RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)  
(preparation and absorption and fluorescence spectra of conjugated  
omers

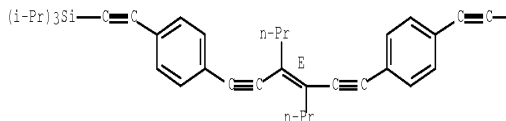
having aromatic (or heteroarom.) and enediyne units alternately in the backbone)

RN 740810-63-3 CAPLUS

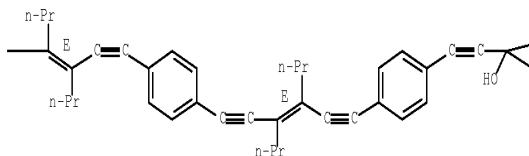


Double bond geometry as shown.

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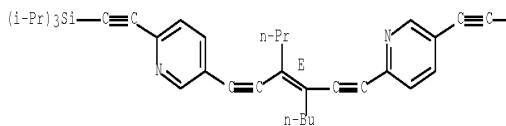
PAGE 1-C



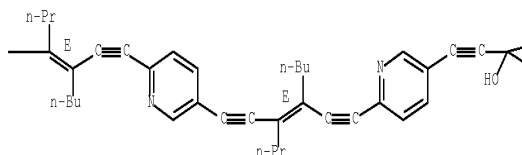
CN 3-Butyn-2-ol, 4-[6-[(3E)-3-butyl-4-[2-[6-[(3E)-3-butyl-4-[2-[6-[(3E)-3-butyl-4-[2-[6-[2-[tris(1-methylethyl)silyl]ethynyl]-3-pyridinyl]ethynyl]-3-hepten-1-yn-1-yl]-3-pyridinyl]ethynyl]-3-hepten-1-yn-1-yl]-3-pyridinyl]ethynyl]-3-hepten-1-yn-1-yl]-3-pyridinyl]-2-methyl- (CA INDEX NAME)

Double bond geometry as shown.

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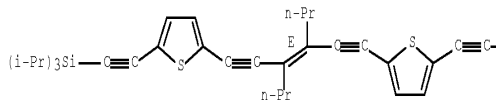
PAGE 1-C



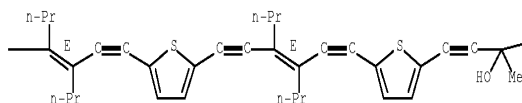
CN 3-Butyn-2-ol, 4-[5-[ (3E)-4-[2-[5-[ (3E)-5-ethyl-4-[2-[5-[ (3E)-5-ethyl-3-propyl-4-[2-[5-[2-[tris (1-methylethyl)silyl]ethynyl]-2-thienyl]ethynyl]-3-penten-1-yn-1-yl]-2-thienyl]ethynyl]-3-propyl-3-penten-1-yn-1-yl]-2-thienyl]ethynyl]-3-propyl-3-hepten-1-yn-1-yl]-2-thienyl]-2-methyl- (CA INDEX NAME)

Double bond geometry as shown.

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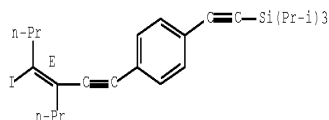




Me

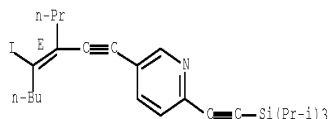
IT 740810-57-5P 740810-53-7P 740810-60-0P  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT  
 (Reactant or reagent)  
 (preparation and absorption and fluorescence spectra of conjugated  
 oligomers  
 having aromatic (or heteroarom.) and enediyne units alternately in the  
 backbone)  
 RN 740810-57-5 CAPLUS  
 CN Benzene, 1-[(3E)-4-iodo-3-propyl-3-hepten-1-yn-1-yl]-4-[2-[tris(1-  
 methylethyl)silyl]ethynyl]- (CA INDEX NAME)

Double bond geometry as shown.



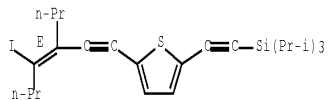
RN 740810-59-7 CAPLUS  
 CN Pyridine, 5-[(3E)-4-iodo-3-propyl-3-octen-1-yn-1-yl]-2-[2-[tris(1-  
 methylethyl)silyl]ethynyl]- (CA INDEX NAME)

Double bond geometry as shown.



RN 740810-60-0 CAPLUS  
 CN Thiophene, 2-[(3E)-4-iodo-3-propyl-3-hepten-1-yn-1-yl]-5-[2-[tris(1-  
 methylethyl)silyl]ethynyl]- (CA INDEX NAME)

Double bond geometry as shown.

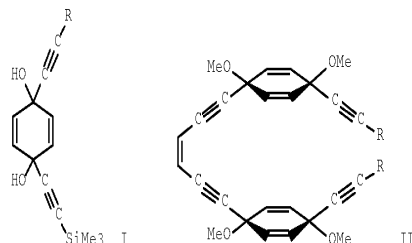


OS.CITING REF COUNT: 20 THERE ARE 20 CAPLUS RECORDS THAT CITE THIS

RECORD (20 CITINGS)

REFERENCE COUNT: 12 THERE ARE 12 CITED REFERENCES AVAILABLE FOR THIS  
 RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 5 OF 11 CAPLUS COPYRIGHT 2009 ACS on STN  
 ACCESSION NUMBER: 2003:491916 CAPLUS [Full-text](#)  
 DOCUMENT NUMBER: 139:395637  
 TITLE: Synthesis of differentially protected/functionalised  
 acetylenic building blocks from p-benzoquinone and  
 their use in the synthesis of new enediynes  
 AUTHOR(S): Sankararaman, Sethuraman; Srinivasan, Manivannan  
 CORPORATE SOURCE: Department of Chemistry, Indian Institute of  
 Technology Madras, Madras, 600 036, India  
 SOURCE: Organic & Biomolecular Chemistry (2003), 1(13),  
 2388-2392  
 CODEN: OBCRAK; ISSN: 1477-0520  
 PUBLISHER: Royal Society of Chemistry  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 OTHER SOURCE(S): CASREACT 139:395637  
 GI



AB Sequential addition of two different lithium acetylides to p-benzoquinone  
 yielded diastereomeric mixts. of 1,4-diethynylcyclohexa-2,5-diene-1,4- diols I  
 [R = (Me2CH)3Si, (EtO)2CH] with different protective/functional groups on the  
 two ethynyl groups. Selective monodeprotection of the di-Me ethers of I to  
 the corresponding terminal acetylenes followed by Pd(0)-mediated coupling with  
 (Z)-1,2-dichloroethene yielded new enediynes II bearing cyclohexa-2,5-diene  
 units.

IT 626235-20-3P  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT  
 (Reactant or reagent)  
 (preparation of cyclohexadienyl enediynes via double addition of  
 functionalized

lithium acetylides to benzoquinone, selective monodeprotection and  
 coupling with dichloroethene)

RN 626235-20-9 CAPLUS  
 CN Silane, [(3Z)-3-hexene-1,5-diene-1,6-diylbis[(cis-1,4-dimethoxy-2,5-  
 cyclohexadiene-1,4-diyl)-2,1-ethynediyl]]bis[tris(1-methylethyl)- (9CI)  
 (CA INDEX NAME)

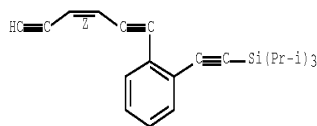
Relative stereochemistry.

Double bond geometry as shown.



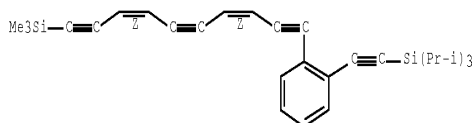
methylethyl)silyl]ethynyl]- (CA INDEX NAME)

Double bond geometry as shown.



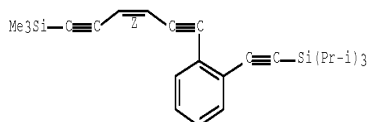
IT 381173-15-58  
RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(deprotection; a combined exptl. and theor. investigation of diatropicity of 3,4,7,8,9,10,13,14-octadehydro[14]annulenes)  
RN 381173-15-5 CAPLUS  
CN Benzene, 1-[(3Z,7Z)-10-(trimethylsilyl)-3,7-decadiene-1,5,9-triyn-1-yl]-2-[2-[tris(1-methylethyl)silyl]ethynyl]- (CA INDEX NAME)

Double bond geometry as shown.



IT 381173-13-3P  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(deprotection; a combined exptl. and theor. investigation of diatropicity of 3,4,7,8,9,10,13,14-octadehydro[14]annulenes)  
RN 381173-13-3 CAPLUS  
CN Benzene, 1-[(3Z)-6-(trimethylsilyl)-3-hexene-1,5-diyn-1-yl]-2-[2-[tris(1-methylethyl)silyl]ethynyl]- (CA INDEX NAME)

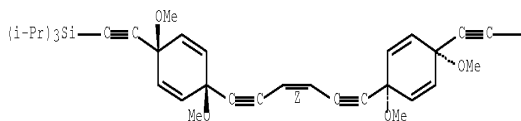
Double bond geometry as shown.



OS.CITING REF COUNT: 31 THERE ARE 31 CAPLUS RECORDS THAT CITE THIS RECORD (33 CITINGS)  
REFERENCE COUNT: 44 THERE ARE 44 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 7 OF 11 CAPLUS COPYRIGHT 2009 ACS on STN

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—Si(Pr-i)3

OS.CITING REF COUNT: 6 THERE ARE 6 CAPLUS RECORDS THAT CITE THIS RECORD (6 CITINGS)  
REFERENCE COUNT: 17 THERE ARE 17 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 6 OF 11 CAPLUS COPYRIGHT 2009 ACS on STN  
ACCESSION NUMBER: 2002:874017 CAPLUS [Full-text](#)  
DOCUMENT NUMBER: 138:72938  
TITLE: Diatropicity of 3,4,7,8,9,10,13,14-Octadehydro[14]annulenes: A Combined Experimental and Theoretical Investigation  
AUTHOR(S): Boydston, Andrew J.; Haley, Michael M.; Williams, Richard Vaughan; Armantrout, John R.  
CORPORATE SOURCE: Department of Chemistry, University of Oregon, Eugene, OR, 97403-1253, USA  
SOURCE: Journal of Organic Chemistry (2002), 67(25), 8812-8819  
CODEN: JOCEAH; ISSN: 0022-3263  
PUBLISHER: American Chemical Society  
DOCUMENT TYPE: Journal  
LANGUAGE: English  
OTHER SOURCE(S): CASREACT 138:72938

AB The synthesis and study of a series of octadehydro[14]annulenes is described. The aromaticity of these annulenes was investigated through examination of exptl. data from arene-fused systems as well as calculated nucleus-independent chemical shifts (NICS) and bond lengths. Benzene ring fusion to the parent system results in a stepwise loss in aromaticity as the number of fused rings is increased from one to two to three. This decrease in annulenic ring current is manifested in the alkene proton chemical shifts (0-2 benzenes) as well as the NICS (0-3 benzenes). Comparison of isomeric thiophene-fused annulenes shows further evidence of ring current competition as these allow for observation of intermittent degrees of delocalization throughout the annulenic core. A consistent relationship between the magnitude of the NICS values and the degree of benzannelation is also observed

IT 482294-19-3P  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(cross-coupling; a combined exptl. and theor. investigation of diatropicity of 3,4,7,8,9,10,13,14-octadehydro[14]annulenes)  
RN 482294-19-9 CAPLUS  
CN Benzene, 1-(3Z)-3-hexene-1,5-diyn-1-yl-2-[2-[tris(1-



ACCESSION NUMBER: 2001:731976 CAPLUS [Full-text](#)  
 DOCUMENT NUMBER: 136:53492  
 TITLE: Diatropicity of Dehydrobenzo[14]annulenes: Comparative Analysis of the Bond-Fixing Ability of Benzene on the Parent 3,4,7,8,9,10,13,14-Octadehydro[14]annulene  
 AUTHOR(S): Boydston, A. J.; Haley, Michael M.  
 CORPORATE SOURCE: Department of Chemistry, University of Oregon, Eugene, OR, 97403-1253, USA  
 SOURCE: Organic Letters (2001), 3(22), 3599-3601  
 CODEN: ORLEF7; ISSN: 1523-7060  
 PUBLISHER: American Chemical Society  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 OTHER SOURCE(S): CASREACT 136:53492

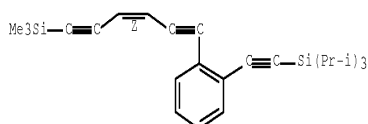
AB We report the synthesis of 3,4,7,8,9,10,13,14-octadehydro[14]annulene and detail a comparative aromaticity study with its benzannulated derivs. (e.g., benzo[e]-3,4,7,8,9,10,13,14-octadehydro[14]annulene and dibenzo[a,e]-3,4,7,8,9,10,13,14-octadehydro[14]annulene).

IT 381173-13-3P 381173-15-5P  
 RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)  
 (intermediate; diatropicity of dehydrobenzoannulenes)

RN 381173-13-3 CAPLUS

CN Benzene, 1-[(3Z)-6-(trimethylsilyl)-3-hexene-1,5-diyn-1-yl]-2-[2-(tris(1-methylethyl)silyl)ethynyl]- (CA INDEX NAME)

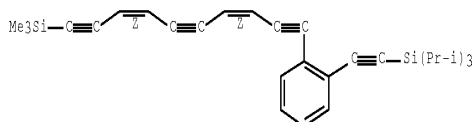
Double bond geometry as shown.



RN 381173-15-5 CAPLUS

CN Benzene, 1-[(3Z,7E)-10-(trimethylsilyl)-3,7-decadiene-1,5,9-triyn-1-yl]-2-[2-(tris(1-methylethyl)silyl)ethynyl]- (CA INDEX NAME)

Double bond geometry as shown.



OS.CITING REF COUNT: 19 THERE ARE 19 CAPLUS RECORDS THAT CITE THIS RECORD (19 CITINGS)

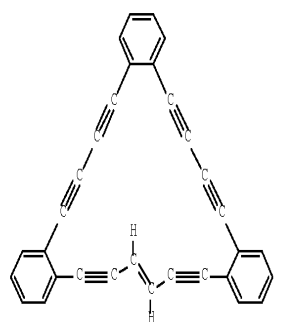
REFERENCE COUNT: 20 THERE ARE 20 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 8 OF 11 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 2001:714296 CAPLUS [Full-text](#)

DOCUMENT NUMBER: 136:69640

TITLE: Synthesis and spectroscopic studies of expanded planar dehydrotribenzo[n]annulenes containing one or two isolated alkene units  
 AUTHOR(S): Wan, W. Brad; Chiechi, Ryan C.; Weakley, Timothy J. R.; Haley, Michael M.  
 CORPORATE SOURCE: Department of Chemistry and the Materials Science Institute, University of Oregon, Eugene, OR, 97403-1253, USA  
 SOURCE: European Journal of Organic Chemistry (2001), (18), 3485-3490  
 CODEN: EJOCFK; ISSN: 1434-193X  
 PUBLISHER: Wiley-VCH Verlag GmbH  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 OTHER SOURCE(S): CASREACT 136:69640  
 GI



AB Dehydrobenzoannulene derivs. containing isolated alkene linkages, e.g., I, were synthesized by combining an in situ Pd/Cu-mediated cross-coupling with an intramol. cyclization strategy. 1H NMR studies of these macrocycles and comparison with related systems verify that highly alkynylated dehydrobenzoannulenes possess weak induced ring currents, indicative of aromatic (4n+2  $\pi$  systems) and antiarom. (4n  $\pi$  systems) behavior, in spite of their large size and extensive benzannulation.

IT 214628-16-7P 214628-17-3P 214628-18-3P  
 363404-34-4P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

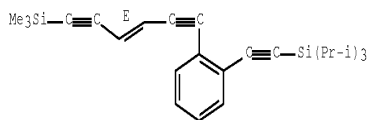
(preparation and spectroscopic studies of expanded planar dehydrotribenzo[n]annulenes containing one or two isolated alkene units)

RN 214628-16-7 CAPLUS

CN Benzene, 1-[(3E)-6-(trimethylsilyl)-3-hexene-1,5-diyn-1-yl]-2-[2-(tris(1-methylethyl)silyl)ethynyl]- (CA INDEX NAME)

Double bond geometry as shown.

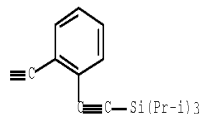




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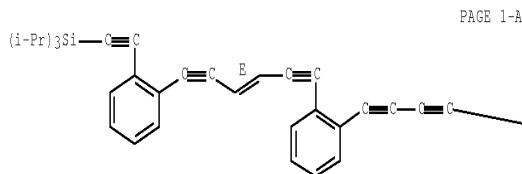
RN 214628-17-8 CAPLUS  
 CN Silane, tris(1-methylethyl)[[2-[(3E)-6-[2-[4-[2-[[tris(1-methylethyl)silyl]ethynyl]phenyl]-1,3-butadiynyl]phenyl]-3-hexene-1,5-diynyl]phenyl]ethynyl]- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

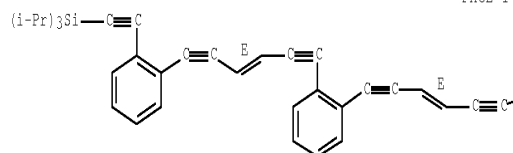


RN 383404-38-4 CAPLUS  
 CN Silane, [1,2-phenylenebis[(3E)-3-hexene-1,5-diyne-6,1-diyl-2,1-phenylene-2,1-ethynediyl]]bis[tris(1-methylethyl)- (9CI) (CA INDEX NAME)

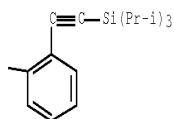
Double bond geometry as shown.



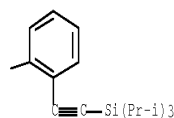
PAGE 1-A



PAGE 1-A



PAGE 1-B

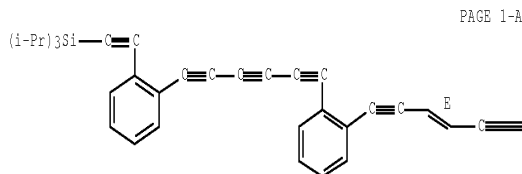


PAGE 1-B

RN 214628-18-9 CAPLUS  
 CN Silane, tris(1-methylethyl)[[2-[6-[2-[(3E)-6-[2-[[tris(1-methylethyl)silyl]ethynyl]phenyl]-3-hexene-1,5-diynyl]phenyl]-1,3,5-hexatriynyl]phenyl]ethynyl]- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

OS.CITING REF COUNT: 10 THERE ARE 10 CAPLUS RECORDS THAT CITE THIS RECORD (10 CITINGS)  
 REFERENCE COUNT: 33 THERE ARE 33 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

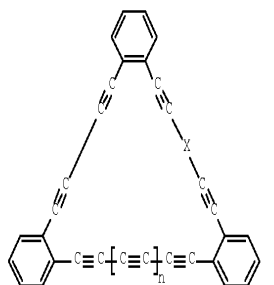


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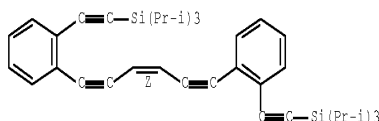
L4 ANSWER 9 OF 11 CAPLUS COPYRIGHT 2009 ACS on STN  
 ACCESSION NUMBER: 2000:832492 CAPLUS [Full-text](#)  
 DOCUMENT NUMBER: 134:310920  
 TITLE: Bis(enediynes) Macrocycles: Synthesis, Reactivity, and Structural Analysis  
 AUTHOR(S): Blanchette, H. S.; Brand, S. C.; Naruse, H.; Weakley, T. J. R.; Haley, M. M.  
 CORPORATE SOURCE: Department of Chemistry, University of Oregon, Eugene, OR, 97403-1253, USA  
 SOURCE: Tetrahedron (2000), 56(49), 9581-9588  
 CODEN: TETRAB; ISSN: 0040-4020  
 PUBLISHER: Elsevier Science Ltd.  
 DOCUMENT TYPE: Journal



LANGUAGE: English  
 OTHER SOURCE(S): CASREACT 134:310920  
 AB The authors describe the syntheses of five macrocycles possessing two enediyne warheads, along with the structural and thermal analyses of these bis(enediyne) compds. The solid-state packing of one of the compds. suggests the possibility for the mol. to undergo a topochem. diacetylene polymerization  
 IT 335378-20-8P  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
 (preparation of bis(enediyne) macrocycles)  
 RN 335378-20-6 CAPLUS  
 CN Silane, [(3Z)-3-hexene-1,5-diyne-1,6-diylbis(2,1-phenylene-2,1-ethynediyl)]bis[tris(1-methylethyl)- (9CI) (CA INDEX NAME)]



Double bond geometry as shown.

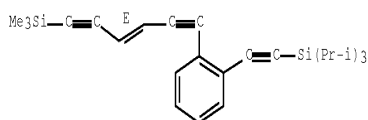


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L4 ANSWER 10 OF 11 CAPLUS COPYRIGHT 2009 ACS on STN  
 ACCESSION NUMBER: 1998:606810 CAPLUS [Full-text](#)  
 DOCUMENT NUMBER: 129:302407  
 ORIGINAL REFERENCE NO.: 129:61683a,61686a  
 TITLE: Synthesis of expanded planar dehydrobenzoannulenes: weakly diatropic, weakly paratropic, or atropic?  
 AUTHOR(S): Wan, W. Brad; Kimball, David B.; Haley, Michael M.  
 CORPORATE SOURCE: Department of Chemistry, University of Oregon, Oregon, 97403-1253, USA  
 SOURCE: Tetrahedron Letters (1998), 39(38), 6795-6798  
 CODEN: TELEAY; ISSN: 0040-4039  
 PUBLISHER: Elsevier Science Ltd.  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 OTHER SOURCE(S): CASREACT 129:302407  
 GI

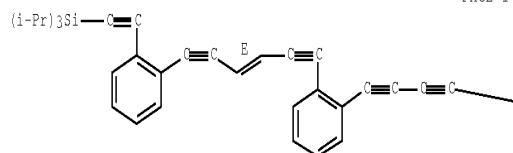
AB Use of a Cu/Pd cross-coupling strategy has led to the synthesis of the first dehydrobenzoannulenes I [X = C.tplbond.C, (E)-CH:CH; n = 0,1] containing triacetylenic linkages. NMR studies of these macrocycles and comparison with other known systems indicate that, in spite of their large size and extensive benzannulation, dehydrobenzoannulenes possess weak induced ring currents.  
 IT 214628-16-7P 214628-17-3P 214628-18-3P  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
 (preparation of expanded planar dehydrobenzoannulenes with triacetylenic linkages)  
 RN 214628-16-7 CAPLUS  
 CN Benzene, 1-[(3E)-6-(trimethylsilyl)-3-hexene-1,5-diyn-1-yl]-2-[2-[tris(1-methylethyl)silyl]ethynyl]- (CA INDEX NAME)

Double bond geometry as shown.



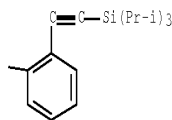
RN 214628-17-8 CAPLUS  
 CN Silane, tris(1-methylethyl)[[2-[(3E)-6-[2-[4-[2-[[tris(1-methylethyl)silyl]ethynyl]phenyl]-1,3-butadiynyl]phenyl]-3-hexene-1,5-diynyl]phenyl]ethynyl]- (9CI) (CA INDEX NAME)

Double bond geometry as shown.





PAGE 1-B

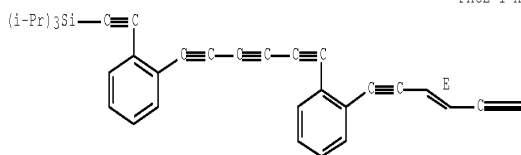


RN 214628-18-9 CAPLUS

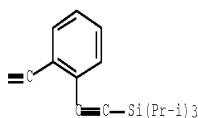
CN Silane, tris(1-methylethyl)[[2-[6-[2-[(3E)-6-[2-[[tris(1-methylethyl)silyl]ethynyl]phenyl]-3-hexene-1,5-diynyl]phenyl]-1,3,5-hexatriynyl]phenyl]ethynyl]- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

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PAGE 1-B



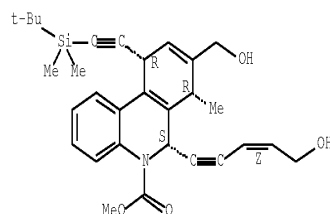
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L4 ANSWER 11 OF 11 CAPLUS COPYRIGHT 2009 ACS on STN  
 ACCESSION NUMBER: 1997:474343 CAPLUS [Full-text](#)  
 DOCUMENT NUMBER: 127:161614  
 ORIGINAL REFERENCE NO.: 127:31327a,31330a  
 TITLE: A new approach to a dynemicin A analog by using an intramolecular Diels-Alder reaction  
 AUTHOR(S): Sakamoto, Yasuharu; Takahashi, Takashi  
 CORPORATE SOURCE: Dep. Chem. Eng., Tokyo Inst. Technol., Tokyo, 152, Japan  
 SOURCE: Synlett (1995), (Spec. Issue), 513-515

CODEN: SYNLES; ISSN: 0936-5214

PUBLISHER: Thieme  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 OTHER SOURCE(S): CASREACT 127:161614  
 AB New synthetic approach to the dynemicin skeleton by using an intramol. Diels-Alder reaction and its diastereoselectivity based on an "MM2 transition-state model" are described.  
 IT 193688-00-5P  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (synthesis of a dynemicin A analog by using an intramol. Diels-Alder reaction)  
 RN 193688-00-5 CAPLUS  
 CN 5(6H)-Phenanthridinecarboxylic acid, 10-[2-[(1,1-dimethylethyl)dimethylsilyl]ethynyl]-7,10-dihydro-8-(hydroxymethyl)-6-[(3Z)-5-hydroxy-3-penten-1-yn-1-yl]-7-methyl-, methyl ester, (6R,7S,10S)-rel- (CA INDEX NAME)

Relative stereochemistry.  
 Double bond geometry as shown.



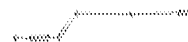
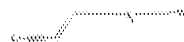
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exact bonds :  
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G1:Cb,Cy,Hy

Match level :  
1:CLASS 2:CLASS 3:CLASS 4:CLASS 5:CLASS 6:CLASS 7:CLASS 9:CLASS

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SAMPLE SCREEN SEARCH COMPLETED - 623 TO ITERATE

100.0% PROCESSED 623 ITERATIONS 2 ANSWERS  
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*  
BATCH \*\*COMPLETE\*\*  
PROJECTED ITERATIONS: 10963 TO 13957  
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C

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L4 20 L3

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YOU HAVE REQUESTED DATA FROM 20 ANSWERS - CONTINUE? Y/(N):y

L4 ANSWER 1 OF 20 CAPLUS COPYRIGHT 2009 ACS on STN  
ACCESSION NUMBER: 2009:76616 CAPLUS [Full-text](#)  
DOCUMENT NUMBER: 150:167710  
TITLE: Push-pull hyperbranched molecules. A theoretical study  
AUTHOR(S): Ramos, Estrella; Guadarrama, Patricia; Teran, Gerardo;  
Fomine, Serguei  
CORPORATE SOURCE: Instituto de Investigaciones en Materiales,  
Universidad Nacional Autonoma de Mexico, Mexico,

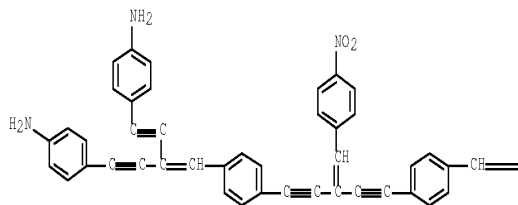
04510, Mex.  
SOURCE: Journal of Physical Organic Chemistry (2009), 22(1),  
9-16  
CODEN: JPOCEE; ISSN: 0894-3230  
PUBLISHER: John Wiley & Sons Ltd.  
DOCUMENT TYPE: Journal  
LANGUAGE: English

AB The electronic properties of the ground state, unrelaxed and relaxed first excited states of push-pull hyperbranched mols. bearing amino and nitro terminal groups have been studied at BB1K/cc-pvdz//HF/6-31g(d), TD-BB1K/cc-pvdz//HF/6-31g(d) and TD-BB1K/cc-pvdz//CIS/6-31g(d) levels of theory, resp. It was demonstrated that dendritic architecture of push-pull mols. favors the charge transfer in the excited state compared to linear mols. The possibility of adopting a plane conformation is an important condition for the charge transfer in an excited state. According to the calcs. 1:1 ratio of donor and acceptor groups is another important precondition for the manifestation of strong charge separation in the excited state. In case of excess of nitro groups over the amino, some of the excitations participating in the S0 → S1 transition favor the charge transfer in the excited state in the opposite directions, thus decreasing the charge separation

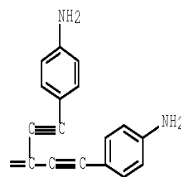
IT 1107616-71-6 1107616-72-7 1107616-73-8  
RL: PRP (Properties)  
(electronic properties of ground state, unrelaxed and relaxed first excited states of push-pull hyperbranched mols. bearing amino and nitro terminal groups)

RN 1107616-71-6 CAPLUS

CN Benzenamine, 4,4'-[3-[[[4-[5-[4-[4-(4-aminophenyl)-2-[2-(4-aminophenyl)ethynyl]-1-buten-3-yn-1-yl]phenyl]-3-[(4-nitrophenyl)methylene]-1,4-pentadiyn-1-yl]phenyl)methylene]-1,4-pentadiyne-1,5-diyl]bis- (CA INDEX NAME)



PAGE 1-A



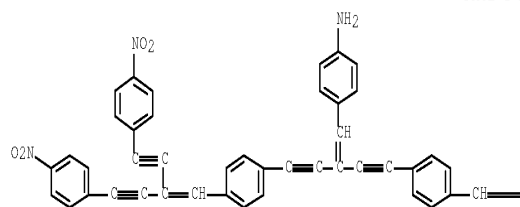
PAGE 1-B

RN 1107616-72-7 CAPLUS

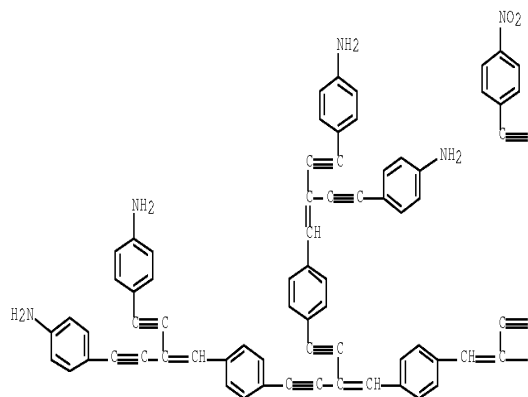


CN Benzenamine, 4,4'-[3-[[4-[5-[4-[4-(4-aminophenyl)-2-[2-(4-aminophenyl)ethynyl]-1-buten-3-yn-1-yl]phenyl]-3-[[4-[4-[4-(4-nitrophenyl)-2-[2-(4-nitrophenyl)ethynyl]-1-buten-3-yn-1-yl]phenyl]-2-[4-[4-(4-nitrophenyl)-2-[2-(4-nitrophenyl)ethynyl]-1-buten-3-yn-1-yl]phenyl]ethynyl]-1-buten-3-yn-1-yl]phenyl]methylene]-1,4-pentadiyn-1-yl]phenyl]methylene]-1,4-pentadiyne-1,5-diyl]bis- (CA INDEX NAME)

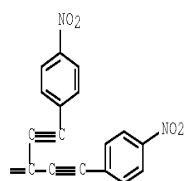
PAGE 1-A



PAGE 1-A



PAGE 1-B



IT 1107616-76-1

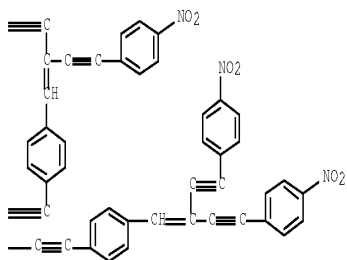
RL: PRP (Properties)

(linear analog; electronic properties of ground state, unrelaxed and relaxed first excited states of push-pull hyperbranched mols. bearing amino and nitro terminal groups)

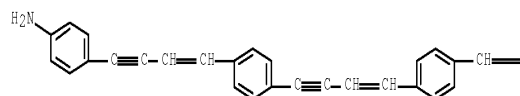
RN 1107616-76-1 CAPLUS

CN Benzenamine, 4-[4-[4-[4-[4-[4-[4-(4-nitrophenyl)-1-buten-3-yn-1-yl]phenyl]-1-buten-3-yn-1-yl]phenyl]-3-buten-1-yn-1-yl]phenyl]-3-buten-1-yn-1-yl]- (CA INDEX NAME)

PAGE 1-B



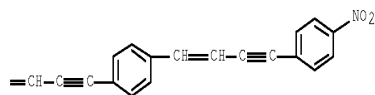
PAGE 1-A



RN 1107616-73-8 CAPLUS

CN Benzenamine, 4-[4-[4-[4-(4-nitrophenyl)-2-[2-(4-nitrophenyl)ethynyl]-1-buten-3-yn-1-yl]phenyl]-2-[2-[4-[4-(4-nitrophenyl)-2-[2-(4-nitrophenyl)ethynyl]-1-buten-3-yn-1-yl]phenyl]ethynyl]-1-buten-3-yn-1-yl]- (CA INDEX NAME)

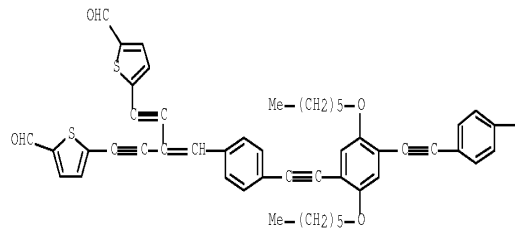
PAGE 1-B





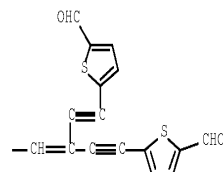
REFERENCE COUNT: 21 THERE ARE 21 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 2 OF 20 CAPLUS COPYRIGHT 2009 ACS on STN  
 ACCESSION NUMBER: 2008:355050 CAPLUS [Full-text](#)  
 DOCUMENT NUMBER: 148:520471  
 TITLE: Tetrafullerene Conjugates for All-Organic Photovoltaics  
 AUTHOR(S): Fernandez, Gustavo; Sanchez, Luis; Veldman, Dirk; Wienk, Martijn M.; Atienza, Carmen; Guldi, Dirk M.; Janssen, Rene A. J.; Martin, Nazario  
 CORPORATE SOURCE: Departamento de Quimica Organica, Facultad de Ciencias Quimicas, Universidad Complutense de Madrid, Madrid, 28040, Spain  
 SOURCE: Journal of Organic Chemistry (2008), 73(8), 3189-3196  
 CODEN: JOCEAH; ISSN: 0022-3263  
 PUBLISHER: American Chemical Society  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 OTHER SOURCE(S): CASREACT 148:520471



AB The synthesis of two new tetrafullerene nanoconjugates in which four C60 units are covalently connected through different  $\pi$ -conjugated oligomers (oligo(p-phenylene ethynylene) and oligo(p-phenylene vinylene)) is described. The photovoltaic response of these C60-based conjugates was evaluated by using them as the only active material in organic solar cells, showing a low photovoltaic performance. Photophys. studies in solution demonstrated a very fast (.apprx.10 ps) deactivation of the singlet excited state of the central core unit to produce both charge-separated species (i.e., C60 $\bullet$ -oligomer $\bullet$ -(C60)3 and C60 centered singlet excited states). The charge-separated state recombines partly to the C60 centered singlet state that undergoes subsequent intersystem crossing. Photophys. studies carried out in films support these data, exhibiting long-lived triplet excited states. For both tetrafullerene arrays, the low yield of long-lived charge carriers in thin films accounts for the limited photovoltaic response. On the contrary, utilizing the oligo(p-phenylene vinylene) centered precursor aldehyde as an electron donor and antennae unit and mixing with the well-known C60 derivative PCBM, the photophys. studies in films show the formation of long-lived charges. The photovoltaic devices constructed from these mixts. showed a relatively high photocurrent of 2 mA/cm<sup>2</sup>. The sharp contrast between the nanoconjugates and the phys. blends tentatively was attributed to improved charge dissociation and the collection of more favorable energy levels in the blends as a result of partial aggregation of both of the components.

IT 1022991-37-2F  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
 (in synthesis of tetrafullerene conjugates for all-organic photovoltaics)  
 RN 1022991-37-2 CAPLUS  
 CN 2-Thiophenecarboxaldehyde, 5,5'-[[2,5-bis(hexyloxy)-1,4-phenylene]bis[2,1-ethynediyl-4,1-phenylene[3-[2-(5-formyl-2-thienyl)ethynyl]-3-buten-1-yne-4,1-diyl]]]bis- (CA INDEX NAME)



OS.CITING REF COUNT: 10 THERE ARE 10 CAPLUS RECORDS THAT CITE THIS RECORD (10 CITINGS)  
 REFERENCE COUNT: 58 THERE ARE 58 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 3 OF 20 CAPLUS COPYRIGHT 2009 ACS on STN  
 ACCESSION NUMBER: 2008:244421 CAPLUS [Full-text](#)  
 DOCUMENT NUMBER: 148:403337  
 TITLE: Triphenylphosphine Incorporation Reactions of Diynyl Complexes Containing a TpRu(NO) Fragment and Isomerization to Ruthenacyclobuta[b]naphthalene  
 AUTHOR(S): Arikawa, Yasuhiro; Asayama, Taiki; Tanaka, Chie; Tashita, Shin-ya; Tsuji, Misako; Ikeda, Kenta; Umakoshi, Keisuke; Onishi, Masayoshi  
 CORPORATE SOURCE: Department of Applied Chemistry, Faculty of Engineering, Nagasaki University, Nagasaki, 852-8521, Japan  
 SOURCE: Organometallics (2008), 27(6), 1227-1233  
 CODEN: ORGND7; ISSN: 0276-7333  
 PUBLISHER: American Chemical Society  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 OTHER SOURCE(S): CASREACT 148:403337  
 AB Nitrosylruthenium arylbutadiynyl complexes having a Tp ligand (Tp = BH(pyzazol-1-yl)3) were prepared, and their reactivities toward PPh3 incorporation in the presence of HBF4·Et2O were described. The PPh3 incorporation of mono(arylbutadiynyl) complex TpRuCl(C.tplbond.C-C.tplbond.C-C6H4Me)(NO) (1) resulted in the  $\beta$ -phosphonioalkenyl complex (E)-



[TpRuCl(CH:C(PPh3)-C.tplbond.C- C6H4Me)(NO)]BF4 (2·BF4), whereas when bis(arylbutadiynyl) TpRu(C.tplbond.C-C.tplbond.C-C6H4Me)2(NO) (3) was treated, mono- and bis(β-phosphonioalkenyl) complexes (E)-[TpRu(C.tplbond.C-C.tplbond.C-C6H4Me)(CH:C(PPh3)-C.tplbond.C- C6H4Me)(NO)]BF4 (4·BF4) and (E,E)-[TpRu(CH:C(PPh3)-C.tplbond.C-C6H4Me)2(NO)](BF4)2 {5·(BF4)2} were obtained depending on the reaction conditions. On the other hand, an unsym. mixed (arylbutadiynyl)(3-hydroxyalkynyl) complex, TpRu(C.tplbond.C-C.tplbond.C-C6H4Me)(C.tplbond.CCPh2(OH))(NO) (6), was allowed to react with PPh3 in the presence of the protic acid to give the α-phosphonioallenyl [TpRu(C.tplbond.C-C.tplbond.C- C6H4Me){C(PPh3):C:Ph2}(NO)]BF4 (7·BF4). Interestingly, thermal isomerization of 7·BF4 to a ruthena-2-PPh3-cyclobuta[b]naphthalene [TpRu(CH(PPh3){3-Ph-8-(MeC6H4-C.tplbond.C)-C10H4}](NO)]BF4 (8·BF4) was observed

IT 55477-27-6P

RL: SPN (Synthetic preparation); PREP (Preparation)  
(triphenylphosphine incorporation reactions of diynyl complexes containing pyrazolylboratoruthenium nitrosyl fragment and isomerization to ruthenacyclobutanaphthalene)

RN 1015477-27-6 CAPLUS

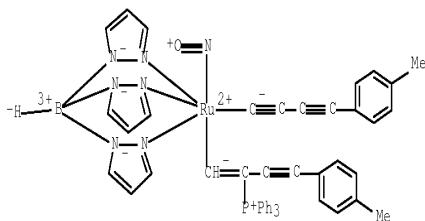
CN Ruthenium(1+), [hydrotris(1H-pyrazolato-κN1)borato(1-)-κN2,κN2',κN2''] [4-(4-methylphenyl)-1,3-butadiyn-1-yl][(1E)-4-(4-methylphenyl)-2-(triphenylphosphonio)-1-buten-3-yn-1-yl]nitrosyl-, (OC-6-24)-, tetrafluoroborate(1-) (1:1) (CA INDEX NAME)

CM 1

CRN 1015477-26-5

CMF C49 H40 B N7 O P Ru

CCI CCS



CM 2

CRN 14874-70-5

CMF B F4

CCI CCS



OS.CITING REF COUNT: 5 THERE ARE 5 CAPLUS RECORDS THAT CITE THIS RECORD (5 CITINGS)

REFERENCE COUNT: 41 THERE ARE 41 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 4 OF 20 CAPLUS COPYRIGHT 2009 ACS ON STN

ACCESSION NUMBER: 2007:1105260 CAPLUS [Full-text](#)

DOCUMENT NUMBER: 148:11306

TITLE: Formation and Structural and Dynamic Features of

Atropisomeric η2-Iminoacyl Zirconium Complexes  
Spies, Patrick; Kehr, Gerald; Kehr, Seda; Froehlich, Roland; Erker, Gerhard

CORPORATE SOURCE: Organisch-Chemisches Institut, Universitaet Muenster, Muenster, 48149, Germany

SOURCE: Organometallics (2007), 26(23), 5612-5620  
CODEN: ORGN7; ISSN: 0276-7333

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 148:11306

AB The Cp2ZrCl[CPh:C(PX2)C.tplbond.CPh] complexes 7a (X = Ph) and 10 (X = C6F5) insert tert-butylisonitrile into the Zr-C(sp2) σ bond to yield the iminoacyl zirconocene complexes, Cp2ZrCl[C(:NCMe3)CPh:C(PX2)C.tplbond.CPh] 13a and 13b. X-ray crystal structure anal. of complexes 13a and 13b revealed a chiral atropisomeric structure with a torsion angle of 74.8(2)° (13a) and 72.9(6)° (13b), resp., around the central iminoacyl/alkenyl C(sp2)-C(sp2) σ bond. In solution an analogous chiral structure is observed. The barrier of interconversion of the enantiomeric atropisomers of 13a and 13b was determined at ΔG.thermod. (327K) = 14.9 ± 0.3 kcal mol-1 (13a) and ΔG.thermod. (325K) = 14.8 ± 0.3 kcal mol-1 (13b) by temperature-dependent dynamic NMR spectroscopy. Reaction of 7a and 10 with methylolithium followed by treatment with B(C6F5)3 gave the corresponding cationic zirconocene complexes Cp2Zr+(THF)[CPh:C(PX2)C.tplbond.CPh] [MeB-(C6F5)3] 12a and 12b. These complexes took up 2 mol equiv of tert-butylisonitrile to yield the cationic N-inside η2-iminoacyl zirconocene systems 14a and 14b as isonitrile adducts. The cationic complexes 14a and 14b are also axially chiral. The barriers of enantiomerization (ΔG.thermod. (288 K) = 13.1 ± 0.3 kcal mol-1 (14a), ΔG.thermod. (293 K) = 13.4 ± 0.3 kcal mol-1 (14b)) were also determined by dynamic NMR spectroscopy.

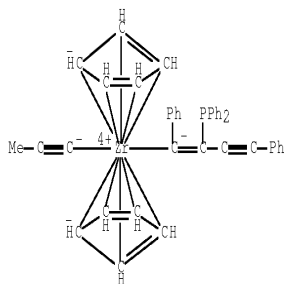
IT 958635-66-0P

RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)  
(crystal structure; isonitrile insertion reaction into neutral and cationic butenynylzirconocene complexes to give atropisomeric iminoacyl zirconocene complexes)

RN 958635-66-0 CAPLUS

CN Zirconium, bis(η5-2,4-cyclopentadien-1-yl){(1E)-2-(diphenylphosphino)-1,4-diphenyl-1-buten-3-yn-1-yl}-1-propyn-1-yl- (CA INDEX NAME)





OS.CITING REF COUNT: 1 THERE ARE 1 CAPLUS RECORDS THAT CITE THIS RECORD (1 CITINGS)  
 REFERENCE COUNT: 60 THERE ARE 60 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 5 OF 20 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 2007:995140 CAPLUS [Full-text](#)

DOCUMENT NUMBER: 147:448227

TITLE: Convenient synthesis of (1-propynyl)arenes through a one-pot double elimination reaction, and their conversion to enynes

AUTHOR(S): An, De-Lie; Zhang, Zhiyang; Orita, Akihiro; Mineyama, Hidetaka; Otera, Junzo

CORPORATE SOURCE: Department of Chemistry, College of Chemistry and Chemical Engineering, Hunan University, Changsha, 410082, Peop. Rep. China

SOURCE: Synlett (2007), (12), 1909-1912

CODEN: SYNLES; ISSN: 0936-5214

PUBLISHER: Georg Thieme Verlag

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 147:448227

AB A series of prop-1-ynyl arenes were prepared by one-pot double elimination reaction of EtSO<sub>2</sub>Ph, aromatic aldehyde, and ClPO(OEt)<sub>2</sub> in THF with a base such as BuLi and tBuOK. A propargyllithium, which was prepared by treatment of propyn-1-yl arene with BuLi in the presence of 1,3-dimethyl-3,4,5,6-tetrahydro-2(1H)-pyrimidinone (DMPU), reacted with aromatic aldehyde, ClPO(OEt)<sub>2</sub> and t-BuOK to afford 4-arylbut-3-en-1-ynyl arene.

Photoluminescence of the enynes thus prepared was recorded both in solution and in the solid state.

IT 951766-78-2R

RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation of propynyl arenes through one-pot double elimination and conversion to enynes)

RN 951766-78-2 CAPLUS

CN Benzene, 1,1'-(1E)-1-buten-3-yne-1,4-diylbis[4-(2-phenylethynyl)- (CA INDEX NAME)

Double bond geometry as shown.

OS.CITING REF COUNT: 2 THERE ARE 2 CAPLUS RECORDS THAT CITE THIS RECORD (2 CITINGS)

REFERENCE COUNT: 24 THERE ARE 24 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 6 OF 20 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 2006:82014 CAPLUS [Full-text](#)

DOCUMENT NUMBER: 144:334159

TITLE: Light harvesting tetrafullerene nanoarray for organic solar cells

AUTHOR(S): Atienza, Carmen M.; Fernandez, Gustavo; Sanchez, Luis; Martin, Nazario; Dantas, Ines Sa; Wienk, Martijn M.; Janssen, Rene A. J.; Rahman, G. M. Aminur; Guldi, Dirk M.

CORPORATE SOURCE: Departamento de Quimica Organica, Facultad de Ciencias Quimicas, Universidad Complutense, Madrid, E-28040, Spain

SOURCE: Chemical Communications (Cambridge, United Kingdom) (2006), (5), 514-516

CODEN: CHCOFS; ISSN: 1359-7345

PUBLISHER: Royal Society of Chemistry

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 144:334159

AB A light absorbing  $\pi$ -conjugated oligomer-tetrafullerene nanoarray was synthesized and its photophys. study reveals an intramol. energy transfer. A photovoltaic device fabricated from this nanoarray and poly(3-hexylthiophene) shows an external quantum efficiency of 15% at 500 nm.

IT 880486-74-8P

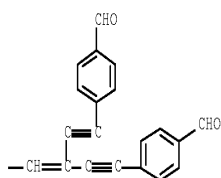
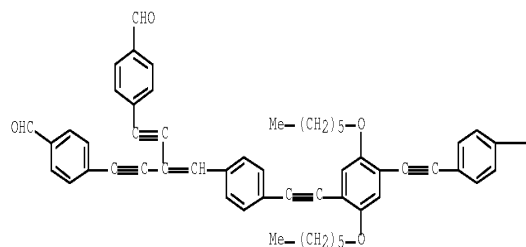
RL: PEP (Physical, engineering or chemical process); PRP (Properties); PUR (Purification or recovery); PYP (Physical process); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); PROC (Process); RACT (Reactant or reagent)

(compound 4; light harvesting tetrafullerene nanoarray for organic solar cells)

RN 880486-74-8 CAPLUS

CN Benzaldehyde, 4,4'-[[2,5-bis(hexyloxy)-1,4-phenylene]bis[2,1-ethynediyl-4,1-phenylene[3-[(4-formylphenyl)ethynyl]-3-buten-1-yne-4,1-diyl]]]bis- (9CI) (CA INDEX NAME)





OS.CITING REF COUNT: 16 THERE ARE 16 CAPLUS RECORDS THAT CITE THIS RECORD (16 CITINGS)

REFERENCE COUNT: 30 THERE ARE 30 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 7 OF 20 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 2005:1004691 CAPLUS [Full-text](#)

DOCUMENT NUMBER: 143:306181

TITLE: Process for preparation of  $\pi$ -conjugated aromatic ring-containing acetylene derivatives as organic electroluminescent devices

INVENTOR(S): Sato, Fumie; Takayama, Yuuki

PATENT ASSIGNEE(S): Nissan Chemical Industries, Ltd., Japan

SOURCE: PCT Int. Appl., 82 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005085176	A1	20050915	WO 2005-JP3950	20050308
W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI,			

NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW

RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

US 20070176164 A1 20070802 US 2007-591950 20070307

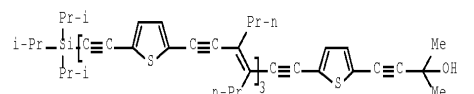
PRIORITY APPLN. INFO.: JP 2004-65446 A 20040309

WO 2005-JP3950 W 20050308

ASSIGNMENT HISTORY FOR US PATENT AVAILABLE IN LSUS DISPLAY FORMAT

OTHER SOURCE(S): MARPAT 143:306181

GI



AB This invention pertains to a method for producing  $\pi$ -conjugated aromatic ring-containing acetylene derivs. via coupling reaction in the presence of palladium and Cu(I) catalysts. For example, the compound I was prepared in a multi-step synthesis in good yield. The title compds. are useful as electroluminescent devices.

IT 864684-11-7P 864684-12-8P 864684-13-9P

864684-15-1P 864684-16-2P 864684-13-5P

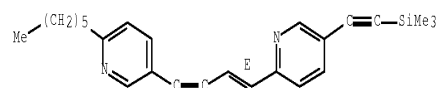
RL: IMF (Industrial manufacture); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(intermediate; preparation of  $\pi$ -conjugated aromatic ring-containing acetylene derivs. as organic electroluminescent devices)

RN 864684-11-7 CAPLUS

CN Pyridine, 2-[(1E)-4-(6-hexyl-3-pyridinyl)-1-buten-3-yn-1-yl]-5-[2-(trimethylsilyl)ethynyl]- (CA INDEX NAME)

Double bond geometry as shown.

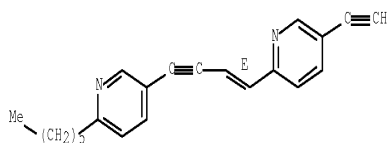


RN 864684-12-8 CAPLUS

CN Pyridine, 5-ethynyl-2-[(1E)-4-(6-hexyl-3-pyridinyl)-1-buten-3-yn-1-yl]- (CA INDEX NAME)

Double bond geometry as shown.

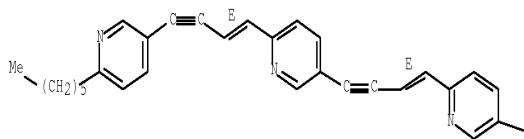




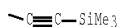
RN 864684-13-9 CAPLUS  
 CN Pyridine, 2-[(1E)-4-(6-hexyl-3-pyridinyl)-1-buten-3-yn-1-yl]-5-[(3E)-4-[5-[2-(trimethylsilyl)ethynyl]-2-pyridinyl]-3-buten-1-yn-1-yl]- (CA INDEX NAME)

Double bond geometry as shown.

PAGE 1-A



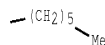
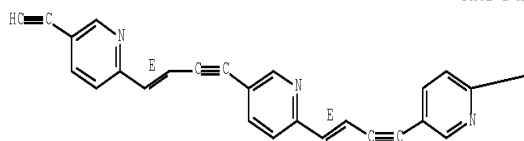
PAGE 1-B



RN 864684-15-1 CAPLUS  
 CN Pyridine, 5-ethynyl-2-[(1E)-4-[6-[(1E)-4-(6-hexyl-3-pyridinyl)-1-buten-3-yn-1-yl]-3-pyridinyl]-1-buten-3-yn-1-yl]- (CA INDEX NAME)

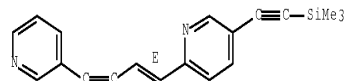
Double bond geometry as shown.

PAGE 1-A



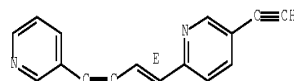
RN 864684-18-4 CAPLUS  
 CN Pyridine, 2-[(1E)-4-(3-pyridinyl)-1-buten-3-yn-1-yl]-5-[2-(trimethylsilyl)ethynyl]- (CA INDEX NAME)

Double bond geometry as shown.



RN 864684-19-5 CAPLUS  
 CN Pyridine, 5-ethynyl-2-[(1E)-4-(3-pyridinyl)-1-buten-3-yn-1-yl]- (CA INDEX NAME)

Double bond geometry as shown.



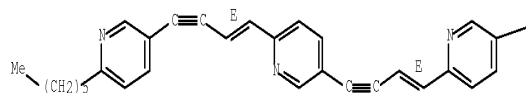
IT 864684-16-2F 864684-17-3F 864684-20-8F  
 RL: DEV (Device component use); IMF (Industrial manufacture); SPN (Synthetic preparation); TEM (Technical or engineered material use); PREP (Preparation); USES (Uses)  
 (preparation of  $\pi$ -conjugated aromatic ring-containing acetylene derivs. as organic electroluminescent devices)

RN 864684-16-2 CAPLUS  
 CN Pyridine, 2-[(1E)-4-[6-[(1E)-4-[6-[(1E)-4-(6-hexyl-3-pyridinyl)-1-buten-3-yn-1-yl]-3-pyridinyl]-1-buten-3-yn-1-yl]-3-pyridinyl]-1-buten-3-yn-1-yl]-5-[2-(trimethylsilyl)ethynyl]- (CA INDEX NAME)

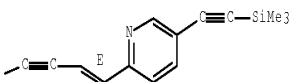
Double bond geometry as shown.



PAGE 1-A

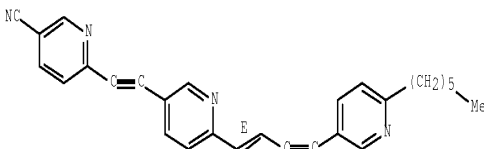


PAGE 1-B



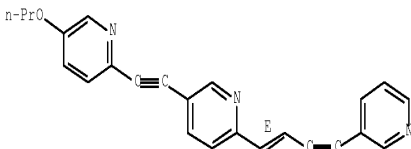
RN 864684-17-3 CAPLUS  
CN 3-Pyridinecarbonitrile, 6-[2-[(1E)-4-(6-hexyl-3-pyridinyl)-1-buten-3-yn-1-yl]-3-pyridinyl]ethynyl]- (CA INDEX NAME)

Double bond geometry as shown.



RN 864684-20-8 CAPLUS  
CN Pyridine, 5-[2-(5-propoxy-2-pyridinyl)ethynyl]-2-[(1E)-4-(3-pyridinyl)-1-buten-3-yn-1-yl]- (CA INDEX NAME)

Double bond geometry as shown.

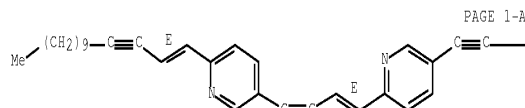


REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 8 OF 20 CAPLUS COPYRIGHT 2009 ACS on STN  
ACCESSION NUMBER: 2004:832644 CAPLUS [Full-text](#)  
DOCUMENT NUMBER: 142:38113

TITLE: Site-Selective Monotitanation of Dialkynylpyridines and Its Application for Preparation of Highly Fluorescent  $\pi$ -Conjugated Oligomers  
AUTHOR(S): Takayama, Yuuki; Hanazawa, Takeshi; Andou, Tomohiro; Muraoka, Kenji; Ohtani, Hiroyuki; Takahashi, Mizuki; Sato, Fumie  
CORPORATE SOURCE: Department of Biomolecular Engineering, Tokyo Institute of Technology, Midori-ku, Yokohama, Kanagawa, 226-8501, Japan  
SOURCE: Organic Letters (2004), 6 (23), 4253-4256  
CODEN: ORLEF7; ISSN: 1523-7060  
PUBLISHER: American Chemical Society  
DOCUMENT TYPE: Journal  
LANGUAGE: English  
OTHER SOURCE(S): CASREACT 142:38113  
AB Reaction of  $\text{Ti}(\text{O}-i\text{-Pr})_4/2i\text{-PrMgCl}$  reagent with 2,n-bis[(trimethylsilyl)ethynyl]pyridines, where n is 3, 4, 5, and 6, or with 3,4-bis[(trimethylsilyl)ethynyl]pyridines, proceeded with excellent site-selectivity to afford the corresponding monotitanated complex. Synthetic application of the reaction was demonstrated by an efficient preparation of  $\pi$ -conjugated oligomers having pyridine and enyne units alternately, which possess intense blue fluorescence emission. Thus, reaction of 2,3-bis[(trimethylsilyl)ethynyl]pyridine with  $\text{Ti}(\text{O}-i\text{-Pr})_4/2i\text{-PrMgCl}$  reagent in  $\text{Et}_2\text{O}$  gave 84% (Z)-2-[2-(trimethylsilyl)ethynyl]-3-[(trimethylsilyl)ethynyl]pyridine.  
IT 805240-17-9P 805240-18-0P  
RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(preparation and site-selective monotitanation of dialkynylpyridines and its application for preparation of highly fluorescent  $\pi$ -conjugated oligomers)  
RN 805240-17-9 CAPLUS  
CN Pyridine, 2-[(1E)-4-[6-(1E)-1-tetradecen-3-yn-1-yl-3-pyridinyl]-1-buten-3-yn-1-yl]-5-[2-(trimethylsilyl)ethynyl]- (CA INDEX NAME)

Double bond geometry as shown.



PAGE 1-A

—SiMe<sub>3</sub>

PAGE 1-B

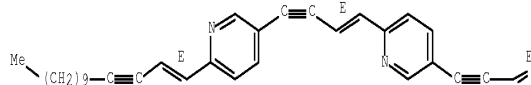
RN 805240-18-0 CAPLUS  
CN Pyridine, 2-[(1E)-4-[6-(1E)-4-[6-(1E)-1-tetradecen-3-yn-1-yl-3-pyridinyl]-1-buten-3-yn-1-yl]-3-pyridinyl]-1-buten-3-yn-1-yl]-5-[2-(trimethylsilyl)ethynyl]- (CA INDEX NAME)

Double bond geometry as shown.

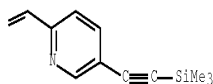


REFERENCE COUNT: 16 THERE ARE 16 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

PAGE 1-A



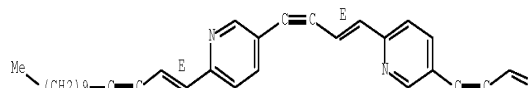
PAGE 1-B



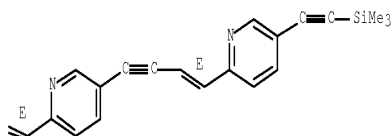
IT 805240-13-1P  
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)  
(preparation and site-selective monofunctionalization of dialkynylpyridines and  
its  
application for preparation of highly fluorescent pi-conjugated oligomers)  
RN 805240-19-1 CAPLUS  
CN Pyridine, 2-[(1E)-4-[6-[(1E)-4-[6-(1E)-1-tetradecen-3-yn-1-yl]-3-  
pyridinyl]-1-buten-3-yn-1-yl]-3-pyridinyl]-1-buten-3-yn-1-yl]-3-pyridinyl]-  
1-buten-3-yn-1-yl]-5-[2-(trimethylsilyl)ethynyl]- (CA INDEX NAME)

Double bond geometry as shown.

PAGE 1-A



PAGE 1-B



OS.CITING REF COUNT: 2 THERE ARE 2 CAPLUS RECORDS THAT CITE THIS RECORD  
(2 CITINGS)

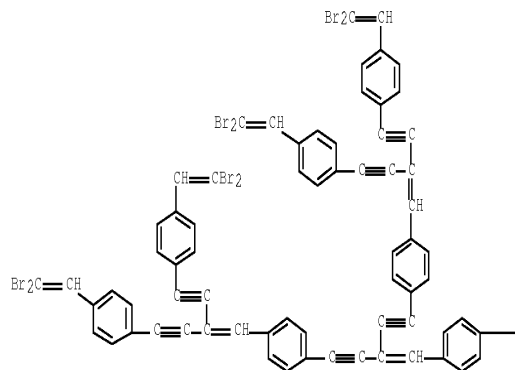
L4 ANSWER 9 OF 20 CAPLUS COPYRIGHT 2009 ACS on STN  
ACCESSION NUMBER: 2004:566840 CAPLUS Full-text  
DOCUMENT NUMBER: 141:261152  
TITLE:  $\pi$ -Conjugated Dendrimers Based on  
Bis(enediynyl)benzene Units  
AUTHOR(S): Hwang, Gil Tae; Kim, Byeang Hyeon  
CORPORATE SOURCE: National Research Laboratory, Department of Chemistry,  
Division of Molecular and Life Sciences, Pohang  
University of Science and Technology, Pohang, 790-784,  
S. Korea  
SOURCE: Organic Letters (2004), 6(16), 2669-2672  
CODEN: ORLEF7; ISSN: 1523-7060  
PUBLISHER: American Chemical Society  
DOCUMENT TYPE: Journal  
LANGUAGE: English

AB We have synthesized a new family of  $\pi$ -conjugated dendrimers that are based on  
bis(enediynyl)benzene units by using both divergent and convergent approaches.  
The compds. at all three generations have strong bluish-green fluorescence,  
especially the third-generation dendrimer, which has the highest extinction  
coefficient and quantum efficiency in this series.

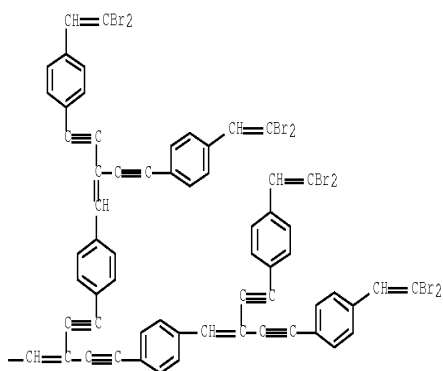
IT 754233-16-4P 754233-13-6P  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT  
(Reactant or reagent)  
(convergent and divergent synthesis of  $\pi$ -conjugated dendrimers based  
on bis(enediynyl)benzene units)

RN 754233-16-4 CAPLUS  
CN Benzene, 1,4-bis[4-[4-[4-(2,2-dibromoethenyl)phenyl]-2-[[4-(2,2-  
dibromoethenyl)phenyl]ethynyl]-1-buten-3-ynyl]phenyl]-2-[[4-[4-(2,2-  
dibromoethenyl)phenyl]-2-[[4-(2,2-dibromoethenyl)phenyl]ethynyl]-1-buten-3-  
ynyl]phenyl]ethynyl]-1-buten-3-ynyl]- (9CI) (CA INDEX NAME)

PAGE 1-A

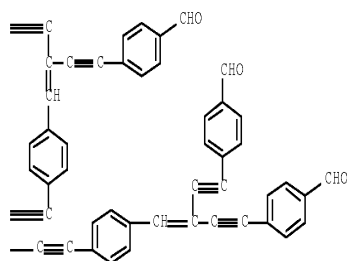






RN 754233-18-6 CAPLUS

CN Benzaldehyde, 4,4'-[[3-[[[4-[[4-[[4-(4-formylphenyl)-2-[(4-formylphenyl)ethynyl]-1-buten-3-ynyl]phenyl]-2-[[4-[[4-(4-formylphenyl)-2-[(4-formylphenyl)ethynyl]-1-buten-3-ynyl]phenyl]ethynyl]-1-buten-3-ynyl]phenyl]methylene]-1,4-pentadiyne-1,5-diyl]bis[4,1-phenylene[3-[(4-formylphenyl)ethynyl]-3-buten-1-yne-4,1-diyl]]]bis- (9CI) (CA INDEX NAME)

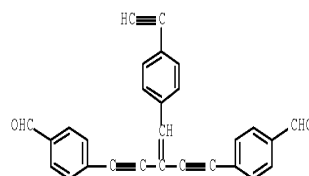
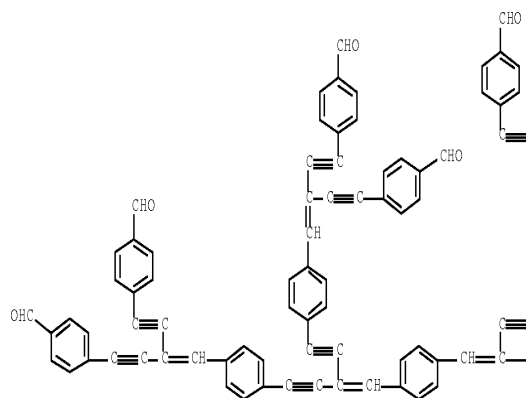


IT 206181-75-1

RL: RCT (Reactant); RACT (Reactant or reagent)  
(in convergent approach; convergent and divergent synthesis of  
π-conjugated dendrimers based on bis(enediynyl)benzene units)

RN 206181-75-1 CAPLUS

CN Benzaldehyde, 4,4'-[3-[(4-ethynylphenyl)methylene]-1,4-pentadiyne-1,5-diyl]bis- (CA INDEX NAME)



OS.CITING REF COUNT: 17 THERE ARE 17 CAPLUS RECORDS THAT CITE THIS RECORD (17 CITINGS)  
REFERENCE COUNT: 33 THERE ARE 33 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 10 OF 20 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 2004:382959 CAPLUS Full-text

DOCUMENT NUMBER: 141:88772

TITLE: Electrochemical and theoretical study of a family of fully conjugated dendritic oligomers

AUTHOR(S): Osorio, Gabriela; Frontana, Carlos; Guadarrama, Patricia; Frontana-Urbe, Bernardo A.

CORPORATE SOURCE: Instituto de Quimica, UNAM, Circuito Exterior Ciudad Universitaria, Mexico, 04510, Mex.

SOURCE: Journal of Physical Organic Chemistry (2004), 17(5), 439-447

CODEN: JPOCEE; ISSN: 0894-3230

PUBLISHER: John Wiley &amp; Sons Ltd.

DOCUMENT TYPE: Journal



LANGUAGE: English

PAGE 1-B

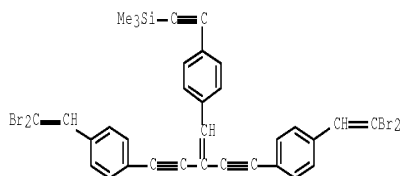
AB Novel dendritic oligomers of  $\beta,\beta$ -dibromo-4-ethynylstyrene and formyl-4-ethynylstyrene were electrochem. and theor. studied to gain a better insight into their redox behavior. Correlations between calculated ionization and exptl. oxidation potentials (anodic peak potentials) were established. The best correlation was obtained when two important effects are considered in the theor. calcs., probing their strong influence: (a) structural re-accommodation in the formed radical cation and (b) solvation effects. The effect of dendritic terminal groups (dibromovinyl and formyl groups) was also analyzed. A different redox behavior was observed for these two terminal groups, presumably due to a difference in their oxidation mechanisms. A global chemical transformation for the oxidation of dibromovinyl-terminated oligomers was proposed, providing a satisfactory explanation of the electrochem. behavior within this family of (presence of adsorptive phenomena). Taking these results into account, it is possible to explain how the cation-radical species formed in these conjugated dendritic oligomers behave when cyclic voltammetry technique is applied.

IT 716327-89-8 716327-90-1 716327-91-2

RL: CPS (Chemical process); FMU (Formation, unclassified); PEP (Physical, engineering or chemical process); PRP (Properties); RCT (Reactant); FORM (Formation, nonpreparative); PROC (Process); RACT (Reactant or reagent)  
(electrochem. and theor. study of fully conjugated dendritic oligomers family)

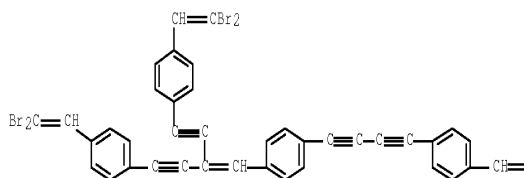
RN 716327-89-8 CAPLUS

CN Silane, [[4-[4-[4-(2,2-dibromoethenyl)phenyl]-2-[[4-(2,2-dibromoethenyl)phenyl]ethynyl]-1-buten-3-ynyl]phenyl]ethynyl]trimethyl-, radical ion(1+) (9CI) (CA INDEX NAME)

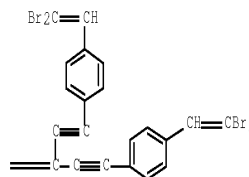


RN 716327-90-1 CAPLUS

CN Benzene, 1,1'-(1,3-butadiyne-1,4-diyl)bis[[4-[4-(2,2-dibromoethenyl)phenyl]-2-[[4-(2,2-dibromoethenyl)phenyl]ethynyl]-1-buten-3-ynyl]-, radical ion(1+) (9CI) (CA INDEX NAME)



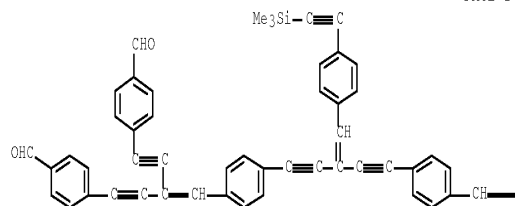
PAGE 1-A



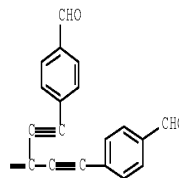
RN 716327-91-2 CAPLUS

CN Benzaldehyde, 4,4'-[[3-[[[4-[(trimethylsilyl)ethynyl]phenyl]methylene]-1,4-pentadiyne-1,5-diyl]bis[4,1-phenylene[3-[(4-formylphenyl)ethynyl]-3-buten-1-yne-4,1-diyl]]]bis-, radical ion(1+) (9CI) (CA INDEX NAME)

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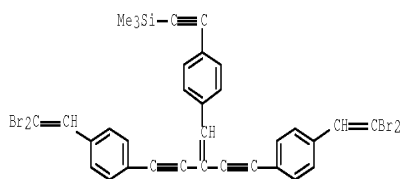
IT 206181-72-8 206181-74-0 206181-76-2

RL: CPS (Chemical process); PEP (Physical, engineering or chemical process); PRP (Properties); RCT (Reactant); PROC (Process); RACT (Reactant or reagent)  
(electrochem. and theor. study of fully conjugated dendritic oligomers family)

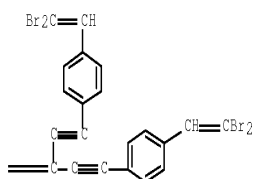
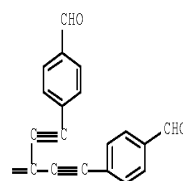
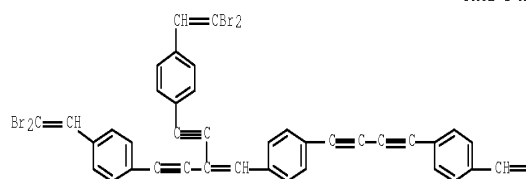
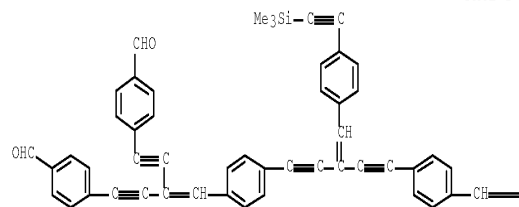
RN 206181-72-8 CAPLUS

CN Silane, [[4-[4-[4-(2,2-dibromoethenyl)phenyl]-2-[[4-(2,2-dibromoethenyl)phenyl]ethynyl]-1-buten-3-ynyl]phenyl]ethynyl]trimethyl-, radical ion(1+) (9CI) (CA INDEX NAME)



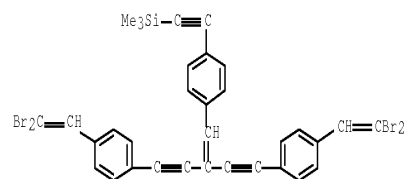


RN 206181-74-0 CAPLUS  
 CN Benzene, 1,1'-(1,3-butadiyne-1,4-diyl)bis[4-[[4-(2,2-dibromoethenyl)phenyl]ethynyl]-1-buten-3-ynyl]- (3CI) (CA INDEX NAME)



RN 206181-76-2 CAPLUS  
 CN Benzaldehyde, 4,4'-[[3-[[4-[(trimethylsilyl)ethynyl]phenyl]methylene]-1,4-pentadiyne-1,5-diyl]bis[4,1-phenylene[3-[(4-formylphenyl)ethynyl]-3-buten-1-yne-4,1-diyl]]]bis- (9CI) (CA INDEX NAME)

IT 717144-23-5 717144-24-6 717144-25-7  
 RL: FMU (Formation, unclassified); PRP (Properties); RCT (Reactant); FORM (Formation, nonpreparative); RACT (Reactant or reagent) (electrochem. and theor. study of fully conjugated dendritic oligomers family)  
 RN 717144-23-5 CAPLUS  
 CN Silane, [[4-[[4-[[4-(2,2-dibromoethenyl)phenyl]-2-[[4-(2,2-dibromoethenyl)phenyl]ethynyl]-1-buten-3-ynyl]phenyl]ethynyl]trimethyl-, radical ion(1-) (9CI) (CA INDEX NAME)



RN 717144-24-6 CAPLUS  
 CN Benzene, 1,1'-(1,3-butadiyne-1,4-diyl)bis[4-[[4-(2,2-dibromoethenyl)phenyl]-2-[[4-(2,2-dibromoethenyl)phenyl]ethynyl]-1-buten-3-ynyl]-, radical ion(1-) (9CI) (CA INDEX NAME)



CN Benzaldehyde, 4,4'-[[3-[[4-[(trimethylsilyl)ethynyl]phenyl]methylene]-1,4-pentadiyne-1,5-diyl]bis[4,1-phenylene]3-[[4-(formylphenyl)ethynyl]-3-buten-1-yne-4,1-diyl]]bis-, radical ion(1-) (9CT) (CA INDEX NAME)

L4 ANSWER 11 of 20 CAPLUS COPYRIGHT 2009 ACS on STN  
ACCESSION NUMBER: 2002:658690 CAPLUS Full-text  
DOCUMENT NUMBER: 137:208374  
TITLE: Manufacturing method of semiconductor device using  
mask pattern having high etching resistance  
INVENTOR(S): Ohuchi, Junko; Sato, Yasuhiko; Shiobara, Eishi;  
Hayashi, Hisataka; Ohiwa, Tokuhisa; Onishi, Yasunobu  
PATENT ASSIGNEE(S): Kabushiki Kaisha Toshiba, Japan  
SOURCE: U.S. Pat. Appl. U.S. Publ., 26 pp.  
CODEN: USXXCO  
DOCUMENT TYPE: Patent  
LANGUAGE: English  
FAMILY ACC. NUM. COUNT: 1  
PATENT INFORMATION:

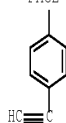
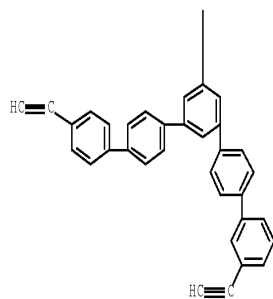
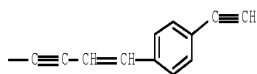
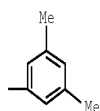
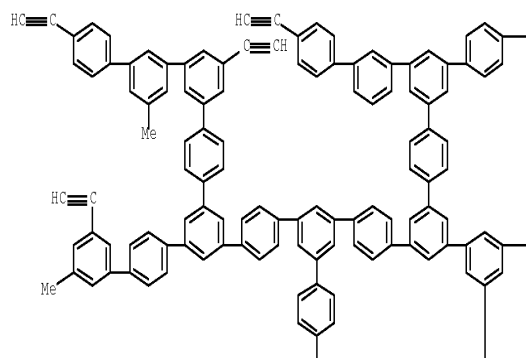
PRIORITY APPLN. INFO.: JP 2000-381410 A 20001215

AB A manufacturing method of semiconductor device comprises (1) forming a mask material having an aromatic ring and carbon content of  $\geq 80\%$  on an object, (2) forming a mask material pattern by etching the mask material to a desired pattern, and (3) etching the object to transfer the mask material pattern as a mask to the object.

RL: TEM (Technical or engineered material use); USES (Uses)  
(semiconductor device mask pattern having high etching resistance  
containing)

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CN      1,'1':3','1''':3','1'''':4''',1''''':3''''',1''''':4''''',1''''':3''''',1''''':  
        ''':4''''',1''''':3''''',1''''':4''''',1''''':3''''',1''''':3''''':3''''':  
        ',1''':1''':4''''',1''''':-Trideciphenyl,  
        4,5''-diethynyl-5''''''''-(4'-ethynyl[1,1'-biphenyl]-4-yl)-5''''''-[3''-  
        ethynyl-5'-(4'-ethynyl[1,1'-biphenyl]-4-yl)[1,1':3',1'':4',1'''-  
        quaterphenyl]-4-yl)-5''''''-(4'-ethynyl-5-[4-(4-ethynylphenyl)-3-buten-1-  
        yl][1,1'-biphenyl]-3-yl)-5''''-(3'-ethynyl-5'-methyl[1,1'-biphenyl]-4-  
        yl)-3''''',5',5''-trimethyl- (9CI) (CA INDEX NAME)
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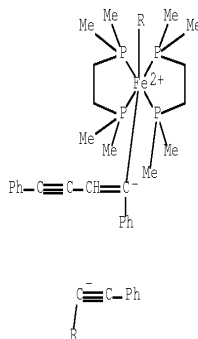
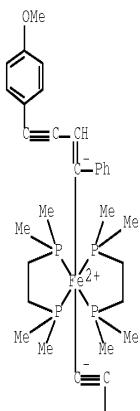
OS.CITING REF COUNT: 8 THERE ARE 8 CAPLUS RECORDS THAT CITE THIS RECORD  
(8 CITINGS)

L4 ANSWER 12 OF 20 CAPLUS COPYRIGHT 2009 ACS on STN  
 ACCESSION NUMBER: 2002:198497 CAPLUS [Full-text](#)  
 DOCUMENT NUMBER: 136:401857  
 TITLE: Acetylide-Bridged Organometallic Oligomers via the Photochemical Metathesis of Methyl-Iron(II) Complexes  
 AUTHOR(S): Field, Leslie D.; Turnbull, Anthony J.; Turner, Peter  
 CORPORATE SOURCE: School of Chemistry, The University of Sydney, Sydney, 2006, Australia  
 SOURCE: Journal of the American Chemical Society (2002), 124(14), 3692-3702  
 CODEN: JACSAT; ISSN: 0002-7863  
 PUBLISHER: American Chemical Society  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 OTHER SOURCE(S): CASREACT 136:401857  
 AB The acetylide Me iron(II) complexes, cis/trans-[Fe(dmpe)2(C.tplbond.CR)(CH3)] (1) and trans-[Fe(depe)2(C.tplbond.CR)(CH3)] (2) (dmpe = 1,2-dimethylphosphinoethane; depe = 1,2-diethylphosphinoethane), were synthesized by transmetalation from the corresponding alkyl halide complexes. Acetylide Me iron(II) complexes were also formed by transmetalation from the chloride complexes, trans-[Fe(dmpe)2(C.tplbond.CR)(Cl)] or trans-[Fe(depe)2(C.tplbond.CR)(Cl)]. The structure of trans-[Fe(dmpe)2(C.tplbond.CC6H5)(CH3)] (1a) was determined by single-crystal x-ray diffraction. The Me acetylide iron complexes, [Fe(dmpe)2(C.tplbond.CR)(CH3)] (1), are thermally stable in the presence of acetylenes; however, under UV irradiation, methane is lost with the formation of a metal bisacetylide. Photochem. metathesis of cis- or trans-[Fe(dmpe)2(CH3)(C.tplbond.CR)] (R = C6H5 (1a), 4-C6H4OCH3 (1b)) with terminal acetylenes was used to selectively synthesize unsym. substituted iron(II) bisacetylide complexes of the type trans-[Fe(dmpe)2(C.tplbond.CR)(C.tplbond.CR')] [R = Ph, R' = Ph (6a), 4-CH3OC6H4 (6b), tBu (6c), SiMe3 (6d), (CH2)4C.tplbond.CH (6e); R = 4-CH3OC6H4, R' = 4-CH3OC6H4, (6g), tBu (6h), (CH2)4C.tplbond.CH (6i), adamantyl (6j)]. The structure of the unsym. iron(II) bisacetylide complex trans-[Fe(dmpe)2(C.tplbond.CC6H5)(C.tplbond.CC6H4OCH3)] (6b) was determined by single-crystal x-ray diffraction. The photochem. metathesis of the bisacetylene, 1,7-octadiyne, with trans-[Fe(dmpe)2(CH3)(C.tplbond.CPh)] (1a), was utilized to synthesize the bridged binuclear species trans,trans-[(C6H5C.tplbond.C)Fe(dmpe)2(μ-C.tplbond.C(CH2)4C.tplbond.C)Fe(dmpe)2(C.tplbond.CC6H5)] (11). The trinuclear species trans,trans,trans-[(C6H5C.tplbond.C)Fe(dmpe)2(μ-C.tplbond.C(CH2)4C.tplbond.C)Fe(dmpe)2(μ-C.tplbond.C(CH2)4C.tplbond.C)Fe(dmpe)2(C.tplbond.CC6H5)] (12) was synthesized by the photochem. reaction of Fe(dmpe)2(C.tplbond.CPh)(C.tplbond.C(CH2)4C.tplbond.CH) (6e) with Fe(dmpe)2(CH3)2. Extended irradiation of the bisacetylide complexes with phenylacetylene resulted in insertion of the terminal alkyne into one of the metal acetylide bonds to give acetylide butenyne complexes. The structure of the acetylide butenyne complex, trans-[Fe(dmpe)2(C.tplbond.CC6H4OCH3)(η1-C(C6H5):CH(C.tplbond.CC6H4OCH3))] (9a) was determined by single-crystal x-ray diffraction.  
 IT 425380-70-7P  
 RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation) (preparation and crystal structure of)  
 RN 425380-70-7 CAPLUS  
 CN Iron, bis[1,2-ethanediy]bis(dimethylphosphine-κP)] [(4-



methoxyphenyl)ethynyl] [(1E)-4- (4-methoxyphenyl)-1-phenyl-1-buten-3-ynyl]-, (OC-6-11)- (9CI) (CA INDEX NAME)

PAGE 1-A



OS.CITING REF COUNT: 13 THERE ARE 13 CAPLUS RECORDS THAT CITE THIS RECORD (13 CITINGS)  
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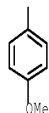
L4 ANSWER 13 OF 20 CAPLUS COPYRIGHT 2009 ACS on STN  
ACCESSION NUMBER: 1999:673316 CAPLUS [Full-text](#)  
DOCUMENT NUMBER: 131:337589  
TITLE: Electronic structure of fully conjugated dendritic oligomers of  $\beta,\beta$ -dibromo-4-ethynyl styrene  
AUTHOR(S): Fomine, Serguei; Fomina, Lioudmila; Guadarrama, Patricia  
CORPORATE SOURCE: Universidad Nacional Autonoma Mexico, Inst de Investigaciones en Materiales, Coyoacan, 04510 CU, Mex.  
SOURCE: THEOCHEM (1999), 488, 207-216  
CODEN: THEODJ; ISSN: 0166-1280  
PUBLISHER: Elsevier Science B.V.  
DOCUMENT TYPE: Journal  
LANGUAGE: English

AB Quantum-mech. calcs. of fully conjugated dendritic oligomers carried out at B3LYP/3-21G//HF/3-21G (d) and B3LYP/3-21G//PM3 levels of theory showed that loose dendritic architecture of  $\beta,\beta$ -dibromo-4-ethynyl styrene oligomers contributes little to the instability and conjugation disruption compared to 1  $\rightarrow$  2 branched polyacetylene, while Br terminal atoms in dendrimers strongly affect the electronic d. distribution in studied mols. On the one hand the bulky bromine atoms decrease the conjugation in Br-terminated dendrimers caused by steric hindrances, on the other hand, highly polarizable bromine atoms reduced significantly adiabatic ionization potentials (IPa) to be up to 1.5 eV lower than corresponding vertical potentials (IPv). Another phenomenon contributing to the reducing of IPa's of all dendrimers is the flattening of mol. geometry accompanying the ionization thus allowing better delocalization of pos. charge over the conjugated system while all aromatic ring except the very outer layer lost their aromaticity becoming essentially quinone by nature.

IT 206181-71-7 206181-72-8 206181-73-9  
206181-74-0 206181-75-1 206181-76-2  
206181-77-3 206181-78-4 206181-79-5

RL: PRP (Properties)  
(electronic structure of fully conjugated dendritic oligomers of  $\beta,\beta$ -dibromo-4-ethynyl styrene)

PAGE 2-A

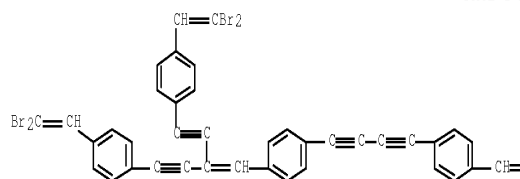
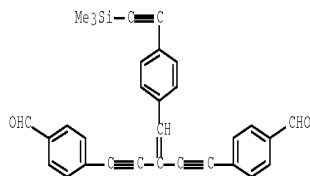


IT 425380-85-4P  
RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation of)  
RN 425380-85-4 CAPLUS  
CN Iron, [(1E)-1,4-diphenyl-1-buten-3-ynyl]bis[1,2-ethanediylbis(dimethylphosphine- $\kappa$ P)](phenylethynyl)-, (OC-6-11)- (9CI) (CA INDEX NAME)



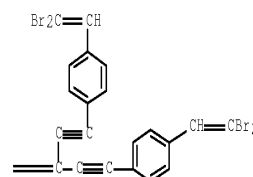
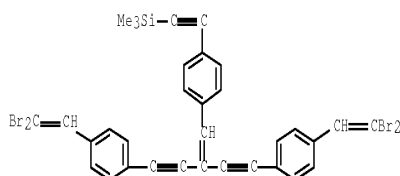
RN 206181-71-7 CAPLUS  
 CN Benzaldehyde, 4,4'-[3-[[4-[(trimethylsilyl)ethynyl]phenyl]methylene]-1,4-pentadiyne-1,5-diyl]bis- (9CI) (CA INDEX NAME)

PAGE 1-A



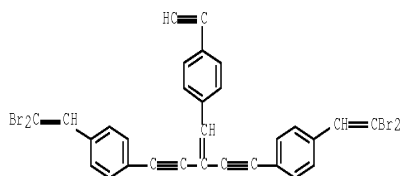
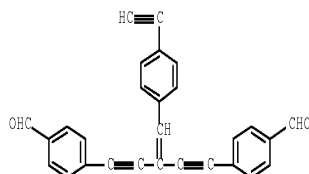
RN 206181-72-8 CAPLUS  
 CN Silane, [[4-[4-(2,2-dibromoethenyl)phenyl]-2-[[4-(2,2-dibromoethenyl)phenyl]ethynyl]-1-buten-3-ynyl]phenyl]ethynyl]trimethyl- (9CI) (CA INDEX NAME)

PAGE 1-B



RN 206181-75-1 CAPLUS  
 CN Benzaldehyde, 4,4'-[3-[[4-(4-ethynylphenyl)methylene]-1,4-pentadiyne-1,5-diyl]bis- (CA INDEX NAME)

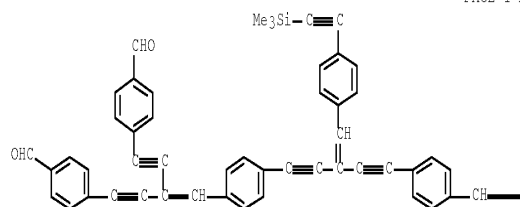
RN 206181-73-9 CAPLUS  
 CN Benzene, 1,1'-[3-[[4-(4-ethynylphenyl)methylene]-1,4-pentadiyne-1,5-diyl]bis[4-(2,2-dibromoethenyl)- (9CI) (CA INDEX NAME)



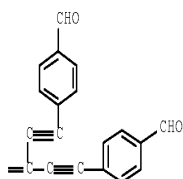
RN 206181-76-2 CAPLUS  
 CN Benzaldehyde, 4,4'-[[3-[[4-[(trimethylsilyl)ethynyl]phenyl]methylene]-1,4-pentadiyne-1,5-diyl]bis[4,1-phenylene[3-[[4-(4-formylphenyl)ethynyl]-3-buten-1-yne-4,1-diyl]]]bis- (9CI) (CA INDEX NAME)

PAGE 1-A

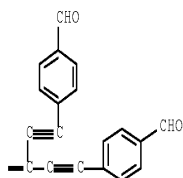
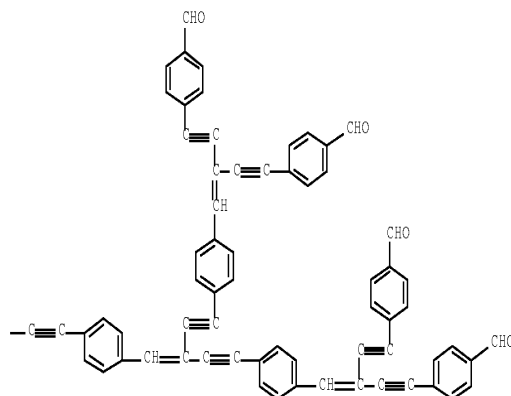
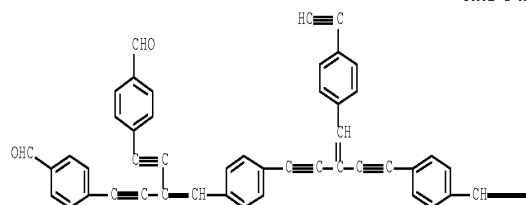
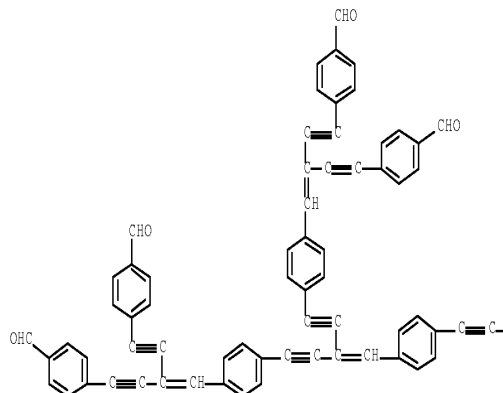
RN 206181-74-0 CAPLUS  
 CN Benzene, 1,1'-[1,3-butadiyne-1,4-diyl]bis[4-[4-[4-(2,2-dibromoethenyl)phenyl]-2-[[4-(2,2-dibromoethenyl)phenyl]ethynyl]-1-buten-3-ynyl]- (9CI) (CA INDEX NAME)







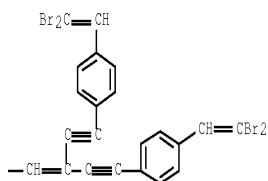
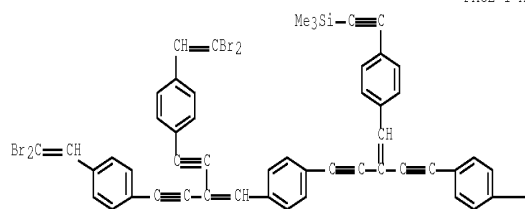
RN 206181-77-3 CAPLUS  
 CN Benzaldehyde, 4,4'-[[3-[(4-ethynylphenyl)methylene]-1,4-pentadiyne-1,5-diyl]bis[4,1-phenylene[3-[(4-formylphenyl)ethynyl]-3-buten-1-yne-4,1-diyl]]bis- (9CI) (CA INDEX NAME)



RN 206181-78-4 CAPLUS  
 CN Benzaldehyde, 4,4'-[1,3-butadiyne-1,4-diylbis[4,1-phenylene[3-[[4-[4-(4-formylphenyl)-2-[(4-formylphenyl)ethynyl]-1-buten-3-ynyl]phenyl]ethynyl]-3-buten-1-yne-4,1-diyl]-4,1-phenylene[3-[(4-formylphenyl)ethynyl]-3-buten-1-yne-4,1-diyl]]bis- (9CI) (CA INDEX NAME)

RN 206181-79-5 CAPLUS  
 CN Silane, [[4-[4-[4-[4-(2,2-dibromoethenyl)phenyl]-2-[[4-(2,2-dibromoethenyl)phenyl]ethynyl]-1-buten-3-ynyl]phenyl]-2-[[4-[4-(2,2-dibromoethenyl)phenyl]-2-[[4-(2,2-dibromoethenyl)phenyl]ethynyl]-1-buten-3-ynyl]phenyl]ethynyl]-1-buten-3-ynyl]phenyl]ethynyl]trimethyl- (9CI) (CA INDEX NAME)





OS.CITING REF COUNT: 2 THERE ARE 2 CAPLUS RECORDS THAT CITE THIS RECORD  
(2 CITINGS)

REFERENCE COUNT: 16 THERE ARE 16 CITED REFERENCES AVAILABLE FOR THIS  
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 14 OF 20 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1999:650836 CAPLUS [Full-text](#)

DOCUMENT NUMBER: 132:16702

TITLE: Theoretical description of luminescent effects in  
 $\beta,\beta$ -di(4'-formylphenylethynyl)-4-ethynylstyrene

AUTHOR(S): Salcedo, R.; Guadarrama, P.; Sansores, L. E.; Fomine, S.; Fomina, L.

CORPORATE SOURCE: Inst. de Investigaciones en Materiales, Inst. de Investigaciones en Materiales, UNAM, Mexico, 04510, Mex.

SOURCE: Materials Research Society Symposium Proceedings (1999), 560(Luminescent Materials), 359-364  
CODEN: MRSPPH; ISSN: 0272-9172

PUBLISHER: Materials Research Society

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Theor. calcons. at HF/6-31 G(d) level were carried out on fully conjugated compds. (4-ethynylbenzaldehyde,  $\beta,\beta$ -dibromo-4-ethynylstyrene,  $\beta,\beta$ -Di(4'-formylphenylethynyl)-4-ethynylstyrene and its dimer) to understand the source of blue emission observed in oligomers of the 1st and 2nd generation in CHCl<sub>3</sub> solns. The frontier orbitals are distributed through the framework of the mols. (benzene rings, double and triple bonds and chromophores). Addnl., a CI approach was applied over  $\beta,\beta$ -Di(4'-formylphenylethynyl)-4-ethynylstyrene

(compound 3) at CIS/6-31 G(d) level to modeling excited states and simulate the UV-visible spectrum exptl. obtained. Calculated transitions corresponded to S<sub>0</sub>→S<sub>1</sub> which are, presumably, responsible for the fluorescence observed

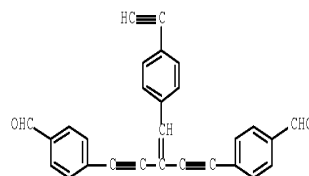
IT 206181-75-1 251479-84-2

RL: PEP (Physical, engineering or chemical process); PRP (Properties); PROC (Process)

(theor. description of luminescent effects in styrene derivs.)

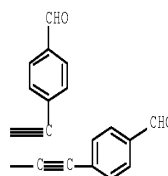
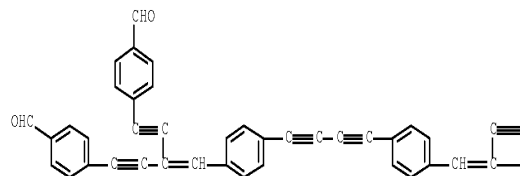
RN 206181-75-1 CAPLUS

CN Benzaldehyde, 4,4'-[3-[(4-ethynylphenyl)methylene]-1,4-pentadiyne-1,5-diyl]bis- (CA INDEX NAME)



RN 251479-84-2 CAPLUS

CN Benzaldehyde, 4,4'-[1,3-butadiyne-1,4-diylbis[4,1-phenylene[3-[(4-formylphenyl)ethynyl]-3-buten-1-yne-4,1-diyl]]]bis- (9CI) (CA INDEX NAME)



OS.CITING REF COUNT: 1 THERE ARE 1 CAPLUS RECORDS THAT CITE THIS RECORD  
(1 CITINGS)

REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS  
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT



L4 ANSWER 15 OF 20 CAPLUS COPYRIGHT 2009 ACS on STN  
 ACCESSION NUMBER: 1998:269262 CAPLUS [Full-text](#)  
 DOCUMENT NUMBER: 128:257221  
 ORIGINAL REFERENCE NO.: 128:50919a,50922a  
 TITLE: Steric Hindrance Facilitated Synthesis of Enynes and Their Intramolecular [4 + 2] Cycloaddition with Alkynes  
 AUTHOR(S): Gonzalez, Juan J.; Francesch, Andres; Cardenas, Diego J.; Echavarren, Antonio M.  
 CORPORATE SOURCE: Departamento de Quimica Organica, Universidad Autonoma de Madrid, Madrid, 28049, Spain  
 SOURCE: Journal of Organic Chemistry (1998), 63(9), 2854-2857  
 CODEN: JOCEAH; ISSN: 0022-3263  
 PUBLISHER: American Chemical Society  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 OTHER SOURCE(S): CASREACT 128:257221

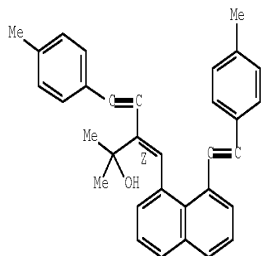
AB The palladium-catalyzed insertion of 1-alkynes into internal alkynes which are bent out of linearity by the interference with a peri or ortho substituent led to enynes regioselectively. The resulting enynes undergo a new type of intramol. thermal cycloaddn., which can be used for the annulation of an aryl ring onto naphthalene derivs. to afford fluranthenes. The cyclization of (E)-1-(1-buten-3-ynyl)-8-ethynyl naphthalene could also be performed in the presence of a Cu(I) catalyst at room temperature

IT 205124-39-6P  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (preparation of enynes and their intramol. [4+2]cycloaddn. with alkynes)

RN 205124-39-6 CAPLUS

CN 4-Pentyn-2-ol, 2-methyl-5-(4-methylphenyl)-3-[[8-[2-(4-methylphenyl)ethynyl]-1-naphthalenyl]methylene]-, (3Z)- (CA INDEX NAME)

Double bond geometry as shown.



OS.CITING REF COUNT: 22 THERE ARE 22 CAPLUS RECORDS THAT CITE THIS RECORD (22 CITINGS)  
 REFERENCE COUNT: 47 THERE ARE 47 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 16 OF 20 CAPLUS COPYRIGHT 2009 ACS on STN  
 ACCESSION NUMBER: 1998:247633 CAPLUS [Full-text](#)  
 DOCUMENT NUMBER: 128:295129  
 ORIGINAL REFERENCE NO.: 128:58501a,58504a  
 TITLE: Synthesis and characterization of well-defined fully conjugated hyperbranched oligomers of  $\beta,\beta$ -dibromo-4-ethynylstyrene

AUTHOR(S): Fomina, Lioudmila; Guadarrama, Patricia; Fomine, Serguei; Salcedo, Roberto; Ogawa, Takeshi  
 CORPORATE SOURCE: Instituto Investigaciones Materiales, Univ. Nacional Autonoma de Mexico, Mexico, 04510, Mex.  
 SOURCE: Polymer (1998), 39(12), 2629-2635  
 CODEN: POLMAG; ISSN: 0032-3861  
 PUBLISHER: Elsevier Science Ltd.  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English

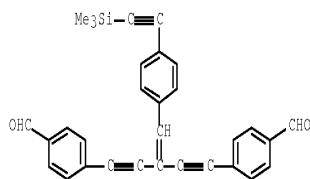
AB Well-defined dendritic oligomers of poly( $\beta,\beta$ -dibromo-4-ethynylstyrene) of the first and second generation were synthesized by a stepwise synthesis, and characterized. NMR and theor. calcons. showed that free rotation around formal single bonds is hampered by conjugation. All of the oligomers were blue emitters with their emission maxima correlating with the number of repeating units. All dendrimers except  $\beta,\beta$ -bis[ $\beta',\beta'$ -di( $\beta'',\beta''$ -dibromostyryl-4"-ethynyl)styryl-4'-ethynyl]-4-ethynylstyrene showed two maxima in the excitation spectra.

IT 206181-71-7P 206181-72-8P 206181-73-3P  
 206181-74-0P 206181-75-1P 206181-76-2P  
 206181-77-3P 206181-78-4P

RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
 (preparation and characterization of conjugated hyperbranched  $\beta,\beta$ -dibromo-4-ethynylstyrene oligomers)

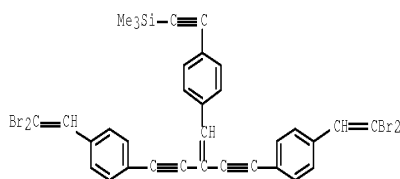
RN 206181-71-7 CAPLUS

CN Benzaldehyde, 4,4'-[3-[[4-[(trimethylsilyl)ethynyl]phenyl]methylene]-1,4-pentadiyne-1,5-diyl]bis- (9CI) (CA INDEX NAME)



RN 206181-72-8 CAPLUS

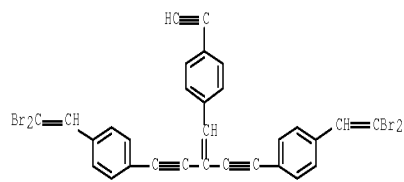
CN Silane, [[4-[4-[4-(2,2-dibromoethenyl)phenyl]-2-[[4-(2,2-dibromoethenyl)phenyl]ethynyl]-1-buten-3-ynyl]phenyl]ethynyl]trimethyl- (9CI) (CA INDEX NAME)



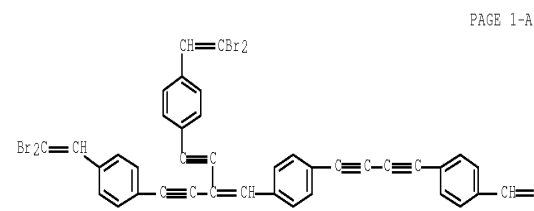
RN 206181-73-9 CAPLUS



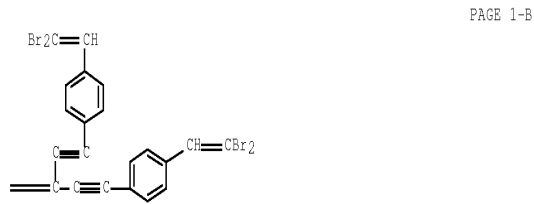
CN Benzene, 1,1'-[3-[(4-ethynylphenyl)methylene]-1,4-pentadiyne-1,5-diyl]bis[4-(2,2-dibromoethenyl)- (9CI) (CA INDEX NAME)



RN 206181-74-0 CAPLUS  
CN Benzene, 1,1'-(1,3-butadiyne-1,4-diyl)bis[4-[4-(2,2-dibromoethenyl)phenyl]-2-[[4-(2,2-dibromoethenyl)phenyl]ethynyl]-1-buten-3-ynyl]- (9CI) (CA INDEX NAME)

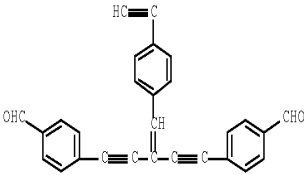


PAGE 1-A

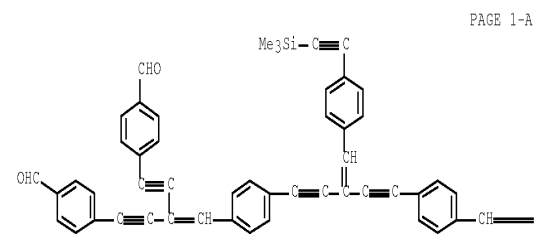


PAGE 1-B

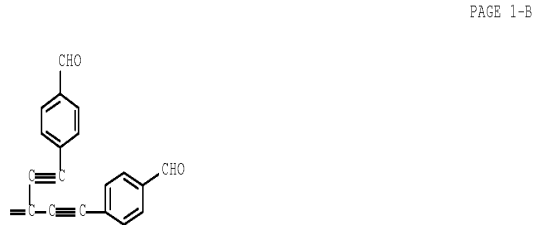
RN 206181-75-1 CAPLUS  
CN Benzaldehyde, 4,4'-[3-[(4-ethynylphenyl)methylene]-1,4-pentadiyne-1,5-diyl]bis- (CA INDEX NAME)



RN 206181-76-2 CAPLUS  
CN Benzaldehyde, 4,4'-[[3-[[4-[(trimethylsilyl)ethynyl]phenyl]methylene]-1,4-pentadiyne-1,5-diyl]bis[4,1-phenylene[3-[(4-formylphenyl)ethynyl]-3-buten-1-yne-4,1-diyl]]]bis- (9CI) (CA INDEX NAME)



PAGE 1-A

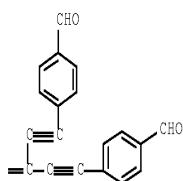
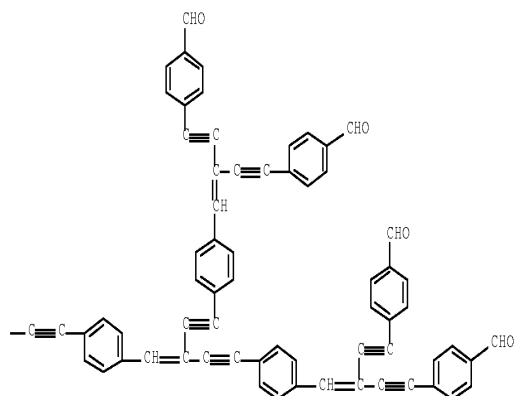
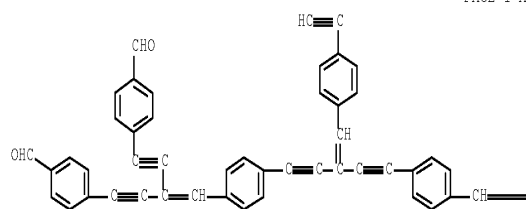


PAGE 1-B

RN 206181-77-3 CAPLUS  
CN Benzaldehyde, 4,4'-[[3-[(4-ethynylphenyl)methylene]-1,4-pentadiyne-1,5-diyl]bis[4,1-phenylene[3-[(4-formylphenyl)ethynyl]-3-buten-1-yne-4,1-diyl]]]bis- (9CI) (CA INDEX NAME)







RN 206181-78-4 CAPLUS

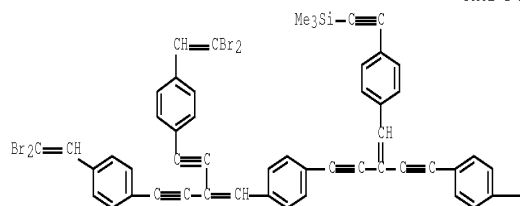
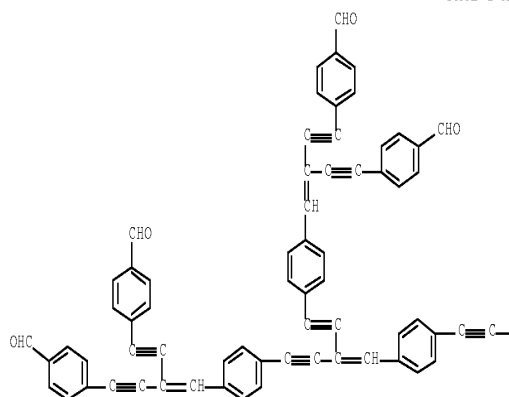
CN Benzaldehyde, 4,4'-[1,3-butadiyne-1,4-diylbis[4,1-phenylene[3-[[4-[4-(4-formylphenyl)-2-[(4-formylphenyl)ethynyl]-1-buten-3-ynyl]phenyl]ethynyl]-3-buten-1-yne-4,1-diyl]-4,1-phenylene[3-[(4-formylphenyl)ethynyl]-3-buten-1-yne-4,1-diyl]]bis- (9CI) (CA INDEX NAME)

IT 206181-79-5P

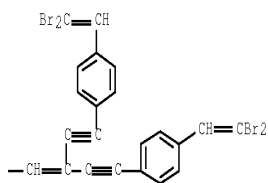
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)  
(preparation and characterization of conjugated hyperbranched  
β,β-dibromo-4-ethynylstyrene oligomers)

RN 206181-79-5 CAPLUS

CN Silane, [[4-[4-[4-[4-(2,2-dibromoethenyl)phenyl]-2-[[4-(2,2-dibromoethenyl)phenyl]ethynyl]-1-buten-3-ynyl]phenyl]-2-[[4-[4-(2,2-dibromoethenyl)phenyl]-2-[[4-(2,2-dibromoethenyl)phenyl]ethynyl]-1-buten-3-ynyl]phenyl]ethynyl]-1-buten-3-ynyl]phenyl]ethynyl]trimethyl- (9CI) (CA INDEX NAME)







OS.CITING REF COUNT: 11 THERE ARE 11 CAPLUS RECORDS THAT CITE THIS RECORD (11 CITINGS)

REFERENCE COUNT: 9 THERE ARE 9 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 17 OF 20 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1996:303100 CAPLUS [Full-text](#)

DOCUMENT NUMBER: 125:11582

ORIGINAL REFERENCE NO.: 125:2539a,2542a

TITLE: Synthesis and polymerization of  $\beta,\beta$ -dibromo-4-ethynylstyrene; preparation of a new polyconjugated, hyperbranched polymer

AUTHOR(S): Fomina, Lioudmila; Salcedo, Roberto

CORPORATE SOURCE: Inst. Investigaciones Materiales, Circuito Exterior, Ciudad Univ., Mexico City, 04510, Mex.

SOURCE: Polymer (1996), 37(9), 1723-1728

CODEN: POLMAG; ISSN: 0032-3861

PUBLISHER: Elsevier

DOCUMENT TYPE: Journal

LANGUAGE: English

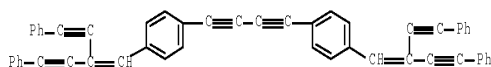
AB The monomer,  $\beta,\beta$ -dibromo-4-ethynylstyrene, was prepared and polymerized by the Heck reaction to give a partially soluble, conjugated hyperbranched polymer. The polymer structure was elucidated using standard spectroscopic techniques and with the aid of model compound synthesis. Theor. calcns. using the AM1 method were carried out and showed that conjugation in the polymer is partially disrupted by twisting of the benzene rings. Both the model compound and the polymer showed luminescence.

IT 171296-95-0P

RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)  
(model compound for dibromoethynylstyrene polymer)

RN 177410-40-1 CAPLUS

CN Benzene, 1,1'-(1,3-butadiene-1,4-diyl)bis[4-(4-phenyl-2-(phenylethynyl)-1-buten-3-ynyl)- (9CI) (CA INDEX NAME)



OS.CITING REF COUNT: 16 THERE ARE 16 CAPLUS RECORDS THAT CITE THIS RECORD (16 CITINGS)

L4 ANSWER 18 OF 20 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1995:946580 CAPLUS [Full-text](#)

DOCUMENT NUMBER: 124:9540

ORIGINAL REFERENCE NO.: 124:2031a,2034a

TITLE: Novel polymers containing discrete conjugated units, produced by the Heck reaction

AUTHOR(S): Fomina, Sergei; Fomina, Lioudmila; Florentino, Hector Quiroz; Mendez, Juan Manuel; Ogawa, Takeshi

CORPORATE SOURCE: Instituto de Investigaciones en Materiales, Universidad Nacional Autonoma de Mexico, Coyoacan, 04510, Mex.

SOURCE: Polymer Journal (Tokyo) (1995), 27(11), 1085-93

CODEN: POLJB8; ISSN: 0032-3896

PUBLISHER: Society of Polymer Science, Japan

DOCUMENT TYPE: Journal

LANGUAGE: English

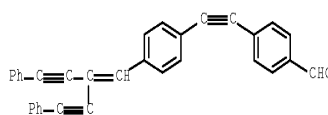
AB Novel monomers and polymers containing arylenevinylideneethynylene groups were synthesized via the Heck reaction. The polymers were amorphous and soluble in common organic solvents. They have Tg .apprx.60°, 5% weight loss at 240-340° and undergo thermal crosslinking at 170-190° with loss of triple bonds. One of the polymers exhibits strong blue luminescence with emission maxima .apprx.380-390 and 470-480 nm with excitation at 320 nm. All polymers show 3rd order NLO susceptibility .apprx.10-10 esu.

IT 171296-95-0P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(intermediate; in preparation of polyacetylene-polyesters)

RN 171296-95-0 CAPLUS

CN Benzaldehyde, 4-[2-[4-(4-phenyl-2-(2-phenylethynyl)-1-buten-3-yn-1-yl)phenyl]ethynyl]- (CA INDEX NAME)

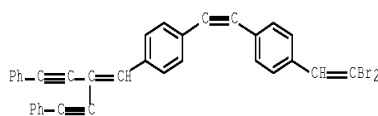


IT 171296-96-1P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(monomer; in preparation of polyacetylene-polyesters)

RN 171296-96-1 CAPLUS

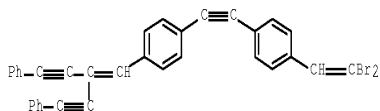
CN Benzene, 1-[2-[4-(2,2-dibromoethenyl)phenyl]ethynyl]-4-[4-phenyl-2-(2-phenylethynyl)-1-buten-3-yn-1-yl]- (CA INDEX NAME)



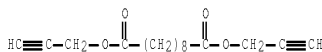
IT 171296-99-4P



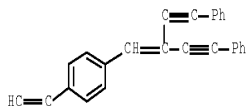
RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(preparation, characterization and properties of)  
RN 171296-99-4 CAPLUS  
CN Decanedioic acid, di-2-propynyl ester, polymer with  
1-[[4-(2,2-dibromoethenyl)phenyl]ethynyl]-4-[4-phenyl-2-(phenylethynyl)-1-buten-3-ynyl]benzene (9CI) (CA INDEX NAME)  
CM 1  
CRN 171296-96-1  
CMF C34 H20 Br2



CM 2  
CRN 93164-22-8  
CMF C16 H22 O4



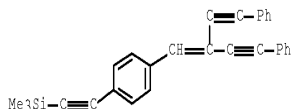
IT 171297-02-2,  $\beta,\beta$ -Bis(phenylethynyl)-4-ethynylstyrene  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(reactant; in preparation of polyacetylene-polyesters)  
RN 171297-02-2 CAPLUS  
CN Benzene, 1-ethynyl-4-[4-phenyl-2-(2-phenylethynyl)-1-buten-3-yn-1-yl]-  
(CA INDEX NAME)



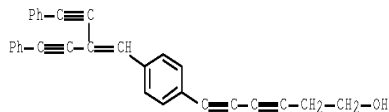
OS.CITING REF COUNT: 11 THERE ARE 11 CAPLUS RECORDS THAT CITE THIS  
RECORD (11 CITINGS)

L4 ANSWER 19 OF 20 CAPLUS COPYRIGHT 2009 ACS on STN  
ACCESSION NUMBER: 1995:642218 CAPLUS [Full-text](#)  
DOCUMENT NUMBER: 123:33763  
ORIGINAL REFERENCE NO.: 123:6259a,6262a

TITLE: Synthesis and molten-state polymerization of some novel conjugated diacetylenes  
AUTHOR(S): Fomina, Lioudmila; Allier, Hector; Fomine, Sergei; Salcedo, Roberto; Ogawa, Takeshi  
CORPORATE SOURCE: Inst. Investigaciones Materiales, Ciudad Univ., Mexico, 04510, Mex.  
SOURCE: Polymer Journal (Tokyo) (1995), 27(6), 591-600  
CODEN: POLJ88; ISSN: 0032-3896  
PUBLISHER: Society of Polymer Science, Japan  
DOCUMENT TYPE: Journal  
LANGUAGE: English  
AB A series of new, highly conjugated diacetylenes, 4-ethynylstilbene derivs., was synthesized and their polymerization was studied. None of them was found to undergo topochem. polymerization in the solid state but they readily polymerized in the molten state to give red transparent and amorphous polymers. All the polymers had an absorption maximum in the visible spectra around 500 nm, and FT-IR data showed the enyne structure of the polymer chain resulted from 1,4-addition  
IT 164467-30-3P  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(in preparation of ethynylstilbene derivative monomers)  
RN 164467-30-5 CAPLUS  
CN Benzene, 1-[4-phenyl-2-(2-phenylethynyl)-1-buten-3-yn-1-yl]-4-[2-(trimethylsilyl)ethynyl]- (CA INDEX NAME)

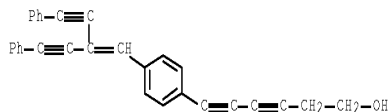


IT 164467-25-3P  
RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation and characterization of polydiacetylenes from ethynylstilbene derivs. in molten state)  
RN 164467-25-8 CAPLUS  
CN 3,5-Hexadiyn-1-ol, 6-[4-[4-phenyl-2-(phenylethynyl)-1-buten-3-ynyl]phenyl]-, homopolymer (9CI) (CA INDEX NAME)  
CM 1  
CRN 164467-20-3  
CMF C30 H20 O





IT 164467-20-3P  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT  
(Reactant or reagent)  
(preparation and polymerization of)  
RN 164467-20-3 CAPLUS  
CN 3,5-Hexadiyn-1-ol, 6-[4-[4-phenyl-2-(2-phenylethynyl)-1-buten-3-yn-1-yl]phenyl]- (CA INDEX NAME)



OS.CITING REF COUNT: 11 THERE ARE 11 CAPLUS RECORDS THAT CITE THIS RECORD (11 CITINGS)

L4 ANSWER 20 OF 20 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1994:522234 CAPLUS [Full-text](#)

DOCUMENT NUMBER: 121:122234

ORIGINAL REFERENCE NO.: 121:21825h,21826a

TITLE: Difluoride derivative and liquid crystal composition containing the same

INVENTOR(S): Yokokoji, Osamu; Irisawa, Jun; Koh, Hidemasa

PATENT ASSIGNEE(S): Asahi Glass Co., Ltd., Japan

SOURCE: PCT Int. Appl., 43 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

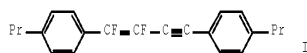
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9405613	A1	19940317	WO 1993-JP1235	19930901
W: US				
RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
EP 628528	A1	19941214	EP 1993-919602	19930901
R: DE, FR, GB, IT				
JP 06263661	A	19940920	JP 1993-219709	19930903
JP 3564711	B2	20040915		
US 5419851	A	19950530	US 1994-211625	19940420
JP 2004292454	A	20041021	JP 2004-115211	20040409
JP 3707493	B2	20051019		
PRIORITY APPLN. INFO.:			JP 1992-263027	A 19920904
			WO 1993-JP1235	W 19930901
			JP 1993-219709	A3 19930903

ASSIGNMENT HISTORY FOR US PATENT AVAILABLE IN LSUS DISPLAY FORMAT

OTHER SOURCE(S): MARPAT 121:122234

GI



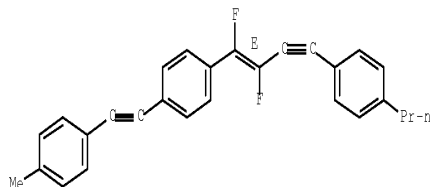
AB Difluoride derivs. represented by the general formula:  
R1(AlY1)mA2CF:CF:tpibond.CA3(Y2A4)nR2 (Al - A4 = trans-1,4-cyclohexylene, 1,4-cyclohexenylene, or 1,4-phenylene wherein ≥1 CH groups of each ring may be substituted by N or ≥1 CH2 groups of the ring may be substituted by O or S; m, n = 0, 1; R1, R2 = C1-10 alkyl, halo, cyano wherein (1) O, CO2, or O2C may be inserted between the C-C bond of alkyl or that between alkyl and ring, (2) a part of the C-C bonds in alkyl is replaced by C:C or C:tpibond.C bond, or (3) one CH2 group in alkyl is replaced by CO group; Y1, Y2 = CO2, O2C, C:tpibond.C, CH2CH2, CH:CH, OCH2, CH2O) are prepared These compds. have low viscosity, are light-stable, and hence can provide a liquid crystal composition having high response speed. Thus, 0.1 mol ClCF:CF2 was blown into THF at -100° followed by adding dropwise 62.1 mL 1.61 M BuLi/hexane, stirring for 30 min, adding dropwise 0.1 mol Me3SiCl, stirring for 1 h, adding dropwise a solution of 4-propylphenyl lithium in THF (prepared from 4-propyliodobenzene and BuLi) at -100°, and stirring for 2 h at 0° to give 75% (Z)-4-PrC6H4CF:CFSiMe3. The latter compound (0.075 mol) was reacted with 0.15 mol KF in aqueous MeCN at 70° for 1 h to give 83% (E)-4-PrC6H4CF:CFH which (0.062 mol) was dissolved in THF, cooled to -78°, and treated dropwise with 38.5 mL 1.61 M BuLi/hexane followed by stirring for 30 min, adding 15.7 g iodine, and stirring at room temperature for 4 h to give 83% (E)-4-PrC6H4CF:CFI. The latter compound (0.051 mol) and 0.051 mol 4-propylphenylacetylene were dissolved in 100 mL Et3N followed by adding Pd(PPh3)2Cl2 and CuI and the resulting mixture was allowed to react at room temperature for 6 h to give 70% diphenyldifluorobutenyne derivative (I). A STN-type liquid crystal display device was prepared from a liquid composition containing 20 weight% I and 80 weight% ZLI-1565 and irradiated with a UV carbon arc lamp for 200 h; new compds. were hardly formed whereas cis-4,4'-bis(n-propyl)difluorostilbene was formed in a liquid crystal composition containing ZLI-1565 and trans-4,4'-bis(n-propyl)difluorostilbene.

IT 156869-08-8P  
RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation of, as liquid crystal with UV stability and low viscosity)

RN 156869-08-8 CAPLUS

CN Benzene, 1-[1,2-difluoro-4-(4-propylphenyl)-1-buten-3-ynyl]-4-[(4-methylphenyl)ethynyl]-, (E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



OS.CITING REF COUNT: 1 THERE ARE 1 CAPLUS RECORDS THAT CITE THIS RECORD (5 CITINGS)

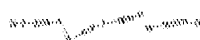
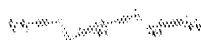
REFERENCE COUNT: 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT



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chain nodes :

2 3 4 5 6 7 8 9 10 11 12 13 14 15 20 24

chain bonds :

2-3 2-24 3-4 4-5 5-6 6-7 7-8 8-9 9-10 10-11 11-12 12-13 13-14 14-15  
15-20

exact/norm bonds :

2-3 2-24 8-9 9-10 15-20

exact bonds :

3-4 4-5 5-6 6-7 7-8 10-11 11-12 12-13 13-14 14-15

G1:Cb,Cy,Hy

G2:C,H,O,N,Cl,Br,F,I

G3:C,H,Si,Cb,Cy,Hy

Match level :

2:CLASS 3:CLASS 4:CLASS 5:CLASS 6:CLASS 7:CLASS 8:CLASS 9:CLASS 10:CLASS  
11:CLASS 12:CLASS 13:CLASS 14:CLASS 15:CLASS 20:CLASS 24:CLASS

L5 STRUCTURE UPLOADED

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FULL SEARCH INITIATED 13:07:29 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - 11729 TO ITERATE

100.0% PROCESSED 11729 ITERATIONS

106 ANSWERS

SEARCH TIME: 00.00.01

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L7 32 L6

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YOU HAVE REQUESTED DATA FROM 32 ANSWERS - CONTINUE? Y/(N):y

L7 ANSWER 1 OF 32 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 2009:1099083 CAPLUS Full-text

DOCUMENT NUMBER: 151:508432

TITLE: Hybrid Conjugated Organic Oligomers Consisting of  
Oligodiacetylene and Thiophene Units: Synthesis and  
Optical Properties

AUTHOR(S): Pilzak, Gregor S.; van Gruijthuijsen, Kitty; van  
Doorn, Reindert H.; van Lagen, Barend; Sudhoelter,  
Ernst J. R.; Zuilhof, Han

CORPORATE SOURCE: Laboratory of Organic Chemistry, Wageningen  
University, Dreijenplein 8, Wageningen, 6703 HB, Neth.

SOURCE: Chemistry--A European Journal (2009), 15(36),  
9085-9096, S9085/1-S9085/19

CODEN: CEUJED; ISSN: 0947-6539

PUBLISHER: Wiley-VCH Verlag GmbH & Co. KGaA

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 151:508432

AB Novel and highly soluble hybrid conjugated organic oligomers consisting of  
oligodiacetylene and thiophene units have been synthesized in high purity  
through iterative and divergent approaches based on a sequence of Sonogashira  
reactions. The series of thiophene-containing oligodiacetylenes and  
homocoupled oligodiacetylenes show, both in solution and in the solid state, a  
strong optical absorption, which is progressively red shifted with increasing  
chain length. The linear correlation of the absorption maximum with the  
inverse of conjugation length (CL = number of double and triple bonds) shows  
that the effective conjugation length of this system is extended up to at  
least CL = 20. Furthermore, absorption measurements of dropcast thin films  
display not only a bathochromic shift of the absorption maxima but also a  
higher wavelength absorption, which is attributed to increased  $\pi$ - $\pi$   
interactions. The wavelength of the maximum fluorescence emission also  
increases with CL, and emission is maximal for oligomers with CL = 7-12  
(fluorescence quantum yield  $\Phi_F$  = .apprx.0.2). Both longer and shorter  
oligomers display marginal emission. The calculated Stokes shifts of these  
planar materials are relatively large (0.4 eV) for all oligomers, and likely  
due to excitation to the S2 state, thus suggesting that the presence of enyne  
moieties dominates the ordering of the lowest excited states. The  
fluorescence lifetimes ( $\tau_F$ ) are short ( $\tau_{Fmax}$  = «1 ns) and closely follow the  
tendency obtained for the fluorescence quantum yield. The anisotropy  
lifetimes show a near-linear increase with CL in line with highly rigid  
oligomers.

IT ~~1192820-79-3P~~

RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)

(synthesis via iterative Sonogashira coupling and optical properties of  
hybrid conjugated organic oligomers consisting of oligodiacetylene and  
thiophene units)

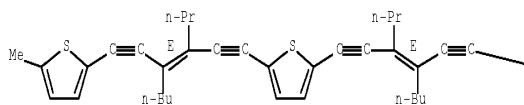
RN 1192820-79-3 CAPLUS

CN INDEX NAME NOT YET ASSIGNED

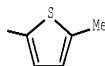
Double bond geometry as shown.



PAGE 1-A



PAGE 1-B



REFERENCE COUNT: 56 THERE ARE 56 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L7 ANSWER 2 OF 32 CAPLUS COPYRIGHT 2009 ACS on STN  
 ACCESSION NUMBER: 2009:76616 CAPLUS [Full-text](#)  
 DOCUMENT NUMBER: 150:167710  
 TITLE: Push-pull hyperbranched molecules. A theoretical study  
 AUTHOR(S): Ramos, Estrella; Guadarrama, Patricia; Teran, Gerardo; Fomine, Serguei  
 CORPORATE SOURCE: Instituto de Investigaciones en Materiales, Universidad Nacional Autonoma de Mexico, Mexico, 04510, Mex.  
 SOURCE: Journal of Physical Organic Chemistry (2009), 22(1), 9-16  
 CODEN: JPOCEE; ISSN: 0894-3230  
 PUBLISHER: John Wiley & Sons Ltd.  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English

AB The electronic properties of the ground state, unrelaxed and relaxed first excited states of push-pull hyperbranched mols. bearing amino and nitro terminal groups have been studied at BB1K/cc-pvdz//HF/6-31g(d), TD-BB1K/cc-pvdz//HF/6-31g(d) and TD-BB1K/cc-pvdz//CIS/6-31g(d) levels of theory, resp. It was demonstrated that dendritic architecture of push-pull mols. favors the charge transfer in the excited state compared to linear mols. The possibility of adopting a plane conformation is an important condition for the charge transfer in an excited state. According to the calcns. 1:1 ratio of donor and acceptor groups is another important precondition for the manifestation of strong charge separation in the excited state. In case of excess of nitro groups over the amino, some of the excitations participating in the S0 → S1 transition favor the charge transfer in the excited state in the opposite directions, thus decreasing the charge separation

IT 1107616-71-6 1107616-72-7 1107616-73-8

RL: PRP (Properties)

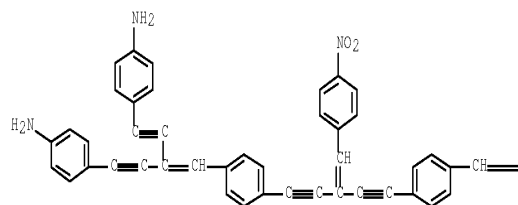
(electronic properties of ground state, unrelaxed and relaxed first excited states of push-pull hyperbranched mols. bearing amino and nitro terminal groups)

RN 1107616-71-6 CAPLUS

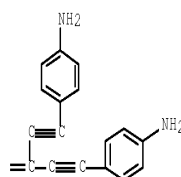
CN Benzenamine, 4,4'-[3-[[4-[5-[4-[4-(4-aminophenyl)-2-[2-(4-aminophenyl)ethynyl]-1-buten-3-yn-1-yl]phenyl]-3-[(4-nitrophenyl)methylene]-1,4-pentadiyn-1-yl]phenyl]methylene]-1,4-pentadiyne-

1,5-diyl]bis- (CA INDEX NAME)

PAGE 1-A



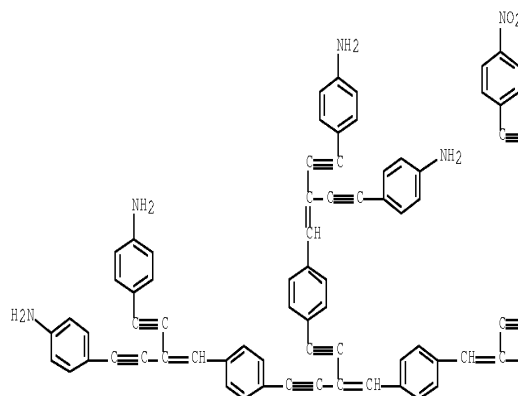
PAGE 1-B



RN 1107616-72-7 CAPLUS

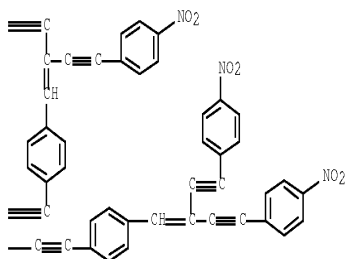
CN Benzenamine, 4,4'-[3-[[4-[5-[4-[4-(4-aminophenyl)-2-[2-(4-aminophenyl)ethynyl]-1-buten-3-yn-1-yl]phenyl]-3-[[4-[4-[4-(4-nitrophenyl)-2-[2-(4-nitrophenyl)ethynyl]-1-buten-3-yn-1-yl]phenyl]-2-[4-[4-(4-nitrophenyl)-2-[2-(4-nitrophenyl)ethynyl]-1-buten-3-yn-1-yl]phenyl]ethynyl]-1-buten-3-yn-1-yl]phenyl]methylene]-1,4-pentadiyn-1-yl]phenyl]methylene]-1,4-pentadiyne-1,5-diyl]bis- (CA INDEX NAME)

PAGE 1-A





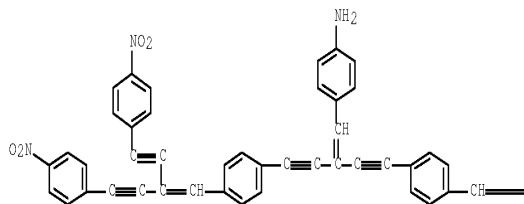
PAGE 1-B



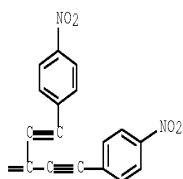
RN 1107616-73-8 CAPLUS

CN Benzenamine, 4-[4-[4-(4-nitrophenyl)-2-[2-(4-nitrophenyl)ethynyl]-1-buten-3-yn-1-yl]phenyl]-2-[2-[4-(4-nitrophenyl)-2-[2-(4-nitrophenyl)ethynyl]-1-buten-3-yn-1-yl]phenyl]ethynyl]-1-buten-3-yn-1-yl]- (CA INDEX NAME)

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IT 1107616-76-1

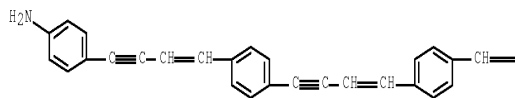
RL: PRP (Properties)

(linear analog; electronic properties of ground state, unrelaxed and relaxed first excited states of push-pull hyperbranched mols. bearing amino and nitro terminal groups)

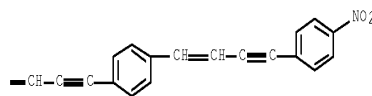
RN 1107616-76-1 CAPLUS

CN Benzenamine, 4-[4-[4-[4-[4-(4-nitrophenyl)-1-buten-3-yn-1-yl]phenyl]-1-buten-3-yn-1-yl]phenyl]-3-buten-1-yn-1-yl]phenyl]-3-buten-1-yn-1-yl]- (CA INDEX NAME)

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PAGE 1-B



REFERENCE COUNT: 21 THERE ARE 21 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L7 ANSWER 3 OF 32 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 2008:355050 CAPLUS [Full-text](#)

DOCUMENT NUMBER: 148:520471

TITLE: Tetrafullerene Conjugates for All-Organic Photovoltaics

AUTHOR(S): Fernandez, Gustavo; Sanchez, Luis; Veldman, Dirk; Wienk, Martijn M.; Atienza, Carmen; Guldi, Dirk M.; Janssen, Rene A. J.; Martin, Nazario

CORPORATE SOURCE: Departamento de Quimica Organica, Facultad de Ciencias Quimicas, Universidad Complutense de Madrid, Madrid, 28040, Spain

SOURCE: Journal of Organic Chemistry (2008), 73(8), 3189-3196 CODEN: JOCEAH; ISSN: 0022-3263

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 148:520471

AB The synthesis of two new tetrafullerene nanoconjugates in which four C60 units are covalently connected through different  $\pi$ -conjugated oligomers (oligo(p-phenylene ethynylene) and oligo(p-phenylene vinylene)) is described. The photovoltaic response of these C60-based conjugates was evaluated by using them as the only active material in organic solar cells, showing a low photovoltaic performance. Photophys. studies in solution demonstrated a very fast (.apprx.10 ps) deactivation of the singlet excited state of the central core unit to produce both charge-separated species (i.e., C60 $\bullet$ -oligomer $\bullet$ +



(C60)3 and C60 centered singlet excited states). The charge-separated state recombines partly to the C60 centered singlet state that undergoes subsequent intersystem crossing. Photophys. studies carried out in films support these data, exhibiting long-lived triplet excited states. For both tetrafullerene arrays, the low yield of long-lived charge carriers in thin films accounts for the limited photovoltaic response. On the contrary, utilizing the oligo(p-phenylene vinylene) centered precursor aldehyde as an electron donor and antennae unit and mixing with the well-known C60 derivative PCBM, the photophys. studies in films show the formation of long-lived charges. The photovoltaic devices constructed from these mixts. showed a relatively high photocurrent of 2 mA/cm2. The sharp contrast between the nanoconjugates and the phys. blends tentatively was attributed to improved charge dissociation and the collection of more favorable energy levels in the blends as a result of partial aggregation of both of the components.

IT 1022991-37-2F

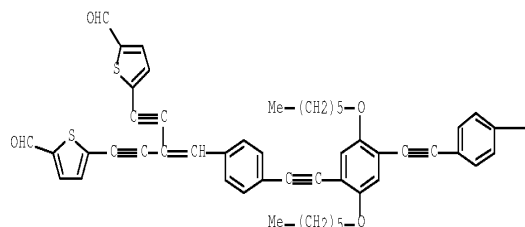
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(in synthesis of tetrafullerene conjugates for all-organic photovoltaics)

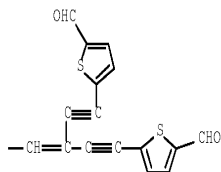
RN 1022991-37-2 CAPLUS

CN 2-Thiophenecarboxaldehyde, 5,5'-[[2,5-bis(hexyloxy)-1,4-phenylene]bis[2,1-ethynediyl-4,1-phenylene[3-[2-(5-formyl-2-thienyl)ethynyl]-3-buten-1-yn-4,1-diyl]]bis- (CA INDEX NAME)

PAGE 1-A



PAGE 1-B

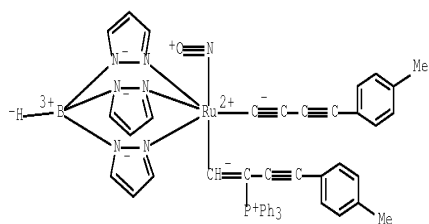


OS.CITING REF COUNT: 10 THERE ARE 10 CAPLUS RECORDS THAT CITE THIS RECORD (10 CITINGS)  
REFERENCE COUNT: 58 THERE ARE 58 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L7 ANSWER 4 OF 32 CAPLUS COPYRIGHT 2009 ACS on STN  
ACCESSION NUMBER: 2008:244421 CAPLUS [Full-text](#)  
DOCUMENT NUMBER: 148:403337  
TITLE: Triphenylphosphine Incorporation Reactions of Diynyl Complexes Containing a TpRu(NO) Fragment and Isomerization to Ruthenacyclobuta[b]naphthalene  
AUTHOR(S): Arikawa, Yasuhiro; Asayama, Taiki; Tanaka, Chie; Tashita, Shin-ya; Tsuji, Misako; Ikeda, Kenta; Umakoshi, Keisuke; Onishi, Masayoshi  
CORPORATE SOURCE: Department of Applied Chemistry, Faculty of Engineering, Nagasaki University, Nagasaki, 852-8521, Japan  
SOURCE: Organometallics (2008), 27(6), 1227-1233  
CODEN: ORGN7; ISSN: 0276-7333  
PUBLISHER: American Chemical Society  
DOCUMENT TYPE: Journal  
LANGUAGE: English  
OTHER SOURCE(S): CASREACT 148:403337  
AB Nitrosylruthenium arylbutadiynyl complexes having a Tp ligand (Tp = BH(pyrazol-1-yl)3) were prepared, and their reactivities toward PPh3 incorporation in the presence of HBF4·Et2O were described. The PPh3 incorporation of mono(arylbutadiynyl) complex TpRuCl(C.tplbond.C-C.tplbond.C-C6H4Me)(NO) (1) resulted in the β-phosphonioalkenyl complex (E)-[TpRuCl(CH:C(PPh3)-C.tplbond.C-C6H4Me)(NO)]BF4 (2·BF4), whereas when bis(arylbutadiynyl) TpRu(C.tplbond.C-C.tplbond.C-C6H4Me)2(NO) (3) was treated, mono- and bis(β-phosphonioalkenyl) complexes (E)-[TpRu(C.tplbond.C-C.tplbond.C-C6H4Me)(CH:C(PPh3)-C.tplbond.C-C6H4Me)(NO)]BF4 (4·BF4) and (E,E)-[TpRu(CH:C(PPh3)-C.tplbond.C-C6H4Me)2(NO)](BF4)2 {5·(BF4)2} were obtained depending on the reaction conditions. On the other hand, an unsym. mixed (arylbutadiynyl)(3-hydroxyalkenyl) complex, TpRu(C.tplbond.C-C.tplbond.C-C6H4Me){C.tplbond.CCPh2(OH)}(NO) (6), was allowed to react with PPh3 in the presence of the protic acid to give the α-phosphonioalkenyl [TpRu(C.tplbond.C-C.tplbond.C-C6H4Me){C(PPh3):C(CPh2)}(NO)]BF4 (7·BF4). Interestingly, thermal isomerization of 7·BF4 to a ruthena-2-PPh3-cyclobuta[b]naphthalene [TpRu(CH(PPh3)[3-Ph-8-(MeC6H4-C.tplbond.C)-ClOH4]}(NO)]BF4 (8·BF4) was observed  
IT 1015477-27-6P  
RL: SPN (Synthetic preparation); PREP (Preparation)  
(triphenylphosphine incorporation reactions of diynyl complexes containing pyrazolylboratoruthenium nitrosyl fragment and isomerization to ruthenacyclobutanaphthalene)  
RN 1015477-27-6 CAPLUS  
CN Ruthenium(1+), [hydrotris(1H-pyrazolato-κN1)borato(1-)-κN2,κN2',κN2''] [4-(4-methylphenyl)-1,3-butadiyn-1-yl][(1E)-4-(4-methylphenyl)-2-(triphenylphosphonio)-1-buten-3-yn-1-yl]nitrosyl-, (OC-6-24)-, tetrafluoroborate(1-) (1:1) (CA INDEX NAME)  
CM 1

CRN 1015477-26-5  
CMF C49 H40 B N7 O P Ru  
CCI CCS





CM 2

CRN 14874-70-5

CMF B F4

CCI CCS



OS.CITING REF COUNT: 5 THERE ARE 5 CAPLUS RECORDS THAT CITE THIS RECORD (5 CITINGS)  
REFERENCE COUNT: 41 THERE ARE 41 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L7 ANSWER 5 OF 32 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 2007:1105260 CAPLUS [Full-text](#)

DOCUMENT NUMBER: 148:11306

TITLE: Formation and Structural and Dynamic Features of

Atropisomeric  $\eta^2$ -Iminoacyl Zirconium Complexes

AUTHOR(S): Spies, Patrick; Kehr, Gerald; Kehr, Seda; Froehlich, Roland; Erker, Gerhard

CORPORATE SOURCE: Organisch-Chemisches Institut, Universitaet Muenster, Muenster, 48149, Germany

SOURCE: Organometallics (2007), 26(23), 5612-5620

CODEN: ORGND7; ISSN: 0276-7333

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 148:11306

AB The  $\text{Cp}_2\text{ZrCl}[\text{CPh}:\text{C}(\text{PX}_2)\text{C.tplbond.CPh}]$  complexes 7a ( $\text{X} = \text{Ph}$ ) and 10 ( $\text{X} = \text{C}_6\text{F}_5$ ) insert tert-butylisocyanide into the  $\text{Zr}-\text{C}(\text{sp}^2)$   $\sigma$  bond to yield the iminoacyl zirconocene complexes,  $\text{Cp}_2\text{ZrCl}[\text{C}(\text{:NCMe}_3)\text{CPh}:\text{C}(\text{PX}_2)\text{C.tplbond.CPh}]$  13a and 13b. X-ray crystal structure anal. of complexes 13a and 13b revealed a chiral atropisomeric structure with a torsion angle of  $74.8(2)^\circ$  (13a) and  $72.9(6)^\circ$  (13b), resp., around the central iminoacyl/alkenyl  $\text{C}(\text{sp}^2)-\text{C}(\text{sp}^2)$   $\sigma$  bond. In solution an analogous chiral structure is observed. The barrier of interconversion of the enantiomeric atropisomers of 13a and 13b was determined at  $\Delta G_{\text{thermod.}}(327\text{K}) = 14.9 \pm 0.3 \text{ kcal mol}^{-1}$  (13a) and  $\Delta G_{\text{thermod.}}(325\text{K}) =$

$14.8 \pm 0.3 \text{ kcal mol}^{-1}$  (13b) by temperature-dependent dynamic NMR spectroscopy. Reaction of 7a and 10 with methylolithium followed by treatment with  $\text{B}(\text{C}_6\text{F}_5)_3$  gave the corresponding cationic zirconocene complexes  $\text{Cp}_2\text{Zr}^+(\text{THF})[\text{CPh}:\text{C}(\text{PX}_2)\text{C.tplbond.CPh}] [\text{MeB}(\text{C}_6\text{F}_5)_3]$  12a and 12b. These complexes took up 2 mol equiv of tert-butylisocyanide to yield the cationic N-inside  $\eta^2$ -iminoacyl zirconocene systems 14a and 14b as isocyanide adducts. The cationic complexes 14a and 14b are also axially chiral. The barriers of enantiomerization ( $\Delta G_{\text{thermod.}}(288\text{K}) = 13.1 \pm 0.3 \text{ kcal mol}^{-1}$  (14a),  $\Delta G_{\text{thermod.}}(293\text{K}) = 13.4 \pm 0.3 \text{ kcal mol}^{-1}$  (14b)) were also determined by dynamic NMR spectroscopy.

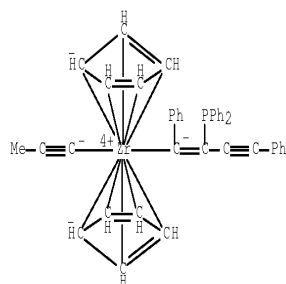
IT 958635-66-00

RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)

(crystal structure; isocyanide insertion reaction into neutral and cationic butenynylzirconocene complexes to give atropisomeric iminoacyl zirconocene complexes)

RN 958635-66-0 CAPLUS

CN Zirconium, bis( $\eta^5$ -2,4-cyclopentadien-1-yl)[(1E)-2-(diphenylphosphino)-1,4-diphenyl-1-buten-3-yn-1-yl]-1-propyn-1-yl- (CA INDEX NAME)



OS.CITING REF COUNT: 1 THERE ARE 1 CAPLUS RECORDS THAT CITE THIS RECORD (1 CITINGS)  
REFERENCE COUNT: 60 THERE ARE 60 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L7 ANSWER 6 OF 32 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 2007:995140 CAPLUS [Full-text](#)

DOCUMENT NUMBER: 147:448227

TITLE: Convenient synthesis of (1-propynyl)arenes through a one-pot double elimination reaction, and their conversion to enynes

AUTHOR(S): An, De-Lie; Zhang, Zhiyang; Orita, Akihiro; Mineyama, Hidetaka; Otera, Junzo

CORPORATE SOURCE: Department of Chemistry, College of Chemistry and Chemical Engineering, Hunan University, Changsha, 410082, Peop. Rep. China

SOURCE: Synlett (2007), (12), 1909-1912

CODEN: SYNLES; ISSN: 0936-5214

PUBLISHER: Georg Thieme Verlag

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 147:448227

AB A series of prop-1-ynyl arenes were prepared by one-pot double elimination reaction of  $\text{EtSO}_2\text{Ph}$ , aromatic aldehyde, and  $\text{ClPO}(\text{OEt})_2$  in THF with a base such



as BuLi and tBuOK. A propargyllithium, which was prepared by treatment of propyn-1-yl arene with BuLi in the presence of 1,3-dimethyl-3,4,5,6-tetrahydro-2(1H)-pyrimidinone (DMPU), reacted with aromatic aldehyde, ClPO(OEt)2 and t-BuOK to afford 4-arylbut-3-en-1-ynyl arene. Photoluminescence of the enynes thus prepared was recorded both in solution and in the solid state.

IT 951766-78-2P

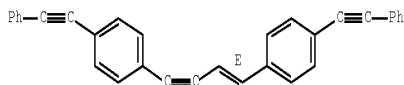
RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation of propynyl arenes through one-pot double elimination and conversion to enynes)

RN 951766-78-2 CAPLUS

CN Benzene, 1,1'-(1E)-1-buten-3-yne-1,4-diylbis[4-(2-phenylethynyl)- (CA INDEX NAME)

Double bond geometry as shown.



OS.CITING REF COUNT: 2 THERE ARE 2 CAPLUS RECORDS THAT CITE THIS RECORD (2 CITINGS)  
REFERENCE COUNT: 24 THERE ARE 24 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L7 ANSWER 7 OF 32 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 2007:46877 CAPLUS [Full-text](#)

DOCUMENT NUMBER: 148:284829

TITLE: Synthesis of smallest unit model of graphite intercalation compound and its possibility

AUTHOR(S): Ogoshi, Sensusuke

CORPORATE SOURCE: Department of Applied Chemistry, Faculty of Engineering, Osaka University, Japan

SOURCE: Asahi Garasu Zaidan Josei Kenkyu Seika Hokoku (2006) 01.03.07/1-01.03.07/8

CODEN: AGSHEN; ISSN: 0919-9179

PUBLISHER: Asahi Garasu Zaidan

DOCUMENT TYPE: Journal; (computer optical disk)

LANGUAGE: Japanese

OTHER SOURCE(S): CASREACT 148:284829

AB Graphite is perhaps the simplest layered structure. Many substances can be intercalated between layers of graphite. Upon intercalation, the graphite layers moved apart somewhat due to the intercalated atom. However, the layers still keep parallel each other which would be the key for the formation of intercalation compds. Thus, compds. having two aromatic rings, which can change the distance between the rings and keep parallel to each other, were designed and synthesized. The target compound was 1,8-bis[6-(1-naphthalenyl)-3-hexene-1,5-diynyl]anthracene.

IT 007602-95-0P

RL: SPN (Synthetic preparation); PREP (Preparation)

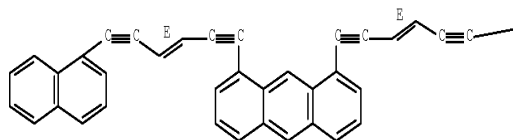
(preparation of bis[(naphthalenyl)hexenediynyl]anthracene (smallest unit model for graphite intercalation compound))

RN 1007602-95-0 CAPLUS

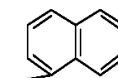
CN Anthracene, 1,8-bis[(3E)-6-(1-naphthalenyl)-3-hexene-1,5-diyn-1-yl]- (CA INDEX NAME)

Double bond geometry as shown.

PAGE 1-A



PAGE 1-B



L7 ANSWER 8 OF 32 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 2006:82014 CAPLUS [Full-text](#)

DOCUMENT NUMBER: 144:334159

TITLE: Light harvesting tetrafullerene nanoarray for organic solar cells

AUTHOR(S): Atienza, Carmen M.; Fernandez, Gustavo; Sanchez, Luis; Martin, Nazario; Dantas, Ines Sa; Wienk, Martijn M.; Janssen, Rene A. J.; Rahman, G. M. Aminur; Guldi, Dirk M.

CORPORATE SOURCE: Departamento de Quimica Organica, Facultad de Ciencias Quimicas, Universidad Complutense, Madrid, E-28040, Spain

SOURCE: Chemical Communications (Cambridge, United Kingdom) (2006), (5), 514-516

CODEN: CHCOFS; ISSN: 1359-7345

PUBLISHER: Royal Society of Chemistry

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 144:334159

AB A light absorbing  $\pi$ -conjugated oligomer-tetrafullerene nanoarray was synthesized and its photophys. study reveals an intramol. energy transfer. A photovoltaic device fabricated from this nanoarray and poly(3-hexylthiophene) shows an external quantum efficiency of 15% at 500 nm.

IT 880486-74-8P

RL: PEP (Physical, engineering or chemical process); PRP (Properties); PUR (Purification or recovery); PYP (Physical process); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); PROC (Process); RACT (Reactant or reagent)

(compound 4; light harvesting tetrafullerene nanoarray for organic solar cells)

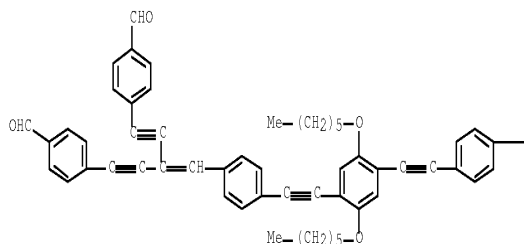
RN 880486-74-8 CAPLUS

CN Benzaldehyde, 4,4'-[2,5-bis(hexyloxy)-1,4-phenylene]bis[2,1-ethynediyl-4,1-phenylene[3-[(4-formylphenyl)ethynyl]-3-buten-1-yne-4,1-diyl]]bis-

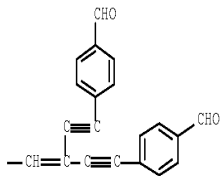


(9CI) (CA INDEX NAME)

PAGE 1-A



PAGE 1-B



OS.CITING REF COUNT: 16 THERE ARE 16 CAPLUS RECORDS THAT CITE THIS  
RECORD (16 CITINGS)  
REFERENCE COUNT: 30 THERE ARE 30 CITED REFERENCES AVAILABLE FOR THIS  
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L7 ANSWER 9 OF 32 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 2005:1004691 CAPLUS Full-text

DOCUMENT NUMBER: 143:306181

TITLE: Process for preparation of  $\pi$ -conjugated aromatic  
ring-containing acetylene derivatives as organic  
electroluminescent devices

INVENTOR(S): Sato, Fumie; Takayama, Yuuki

PATENT ASSIGNEE(S): Nissan Chemical Industries, Ltd., Japan

SOURCE: PCT Int. Appl., 82 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: Japanese

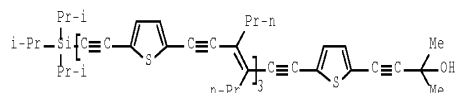
FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005085176	A1	20050915	WO 2005-JP3950	20050308
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH,				

CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD,  
GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC,  
LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI,  
NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM,  
SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW  
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM,  
AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK,  
EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, L7, LU, MC, NL, PL, PT,  
RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML,  
MR, NE, SN, TD, TG

US 20070176164 A1 20070802 US 2007-591950 20070307  
PRIORITY APPLN. INFO.: JP 2004-65446 A 20040309  
WO 2005-JP3950 W 20050308  
ASSIGNMENT HISTORY FOR US PATENT AVAILABLE IN LSUS DISPLAY FORMAT  
OTHER SOURCE(S): MARPAT 143:306181  
GI



AB This invention pertains to a method for producing  $\pi$ -conjugated aromatic ring-  
containing acetylene derivs. via coupling reaction in the presence of  
palladium and Cu(I) catalysts. For example, the compound I was prepared in a  
multi-step synthesis in good yield. The title compds. are useful as  
electroluminescent devices.

IT 740810-64-4F 740810-65-5F 740810-67-7F  
740810-68-8F 740810-69-9F 740810-70-0F  
740810-71-1F 740810-72-2F 740810-73-3F  
740810-74-4F 740810-75-5F 740810-76-6F  
740810-77-7F 740810-78-8F 740810-79-9F  
740810-80-0F 740810-81-1F 740810-82-2F

RL: IMF (Industrial manufacture); RCT (Reactant); SPN (Synthetic  
preparation); PREP (Preparation); RACT (Reactant or reagent)

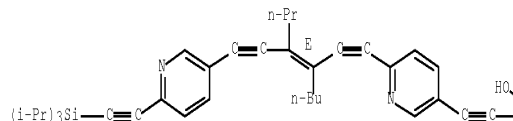
(intermediate; preparation of  $\pi$ -conjugated aromatic ring-containing  
acetylene  
derivs. as organic electroluminescent devices)

RN 740810-64-4 CAPLUS

CN 3-Butyn-2-ol, 4-[6-[(3E)-3-butyl-4-[2-[6-[2-[tris(1-  
methylethyl)silyl]ethynyl]-3-pyridinyl]ethynyl]-3-hepten-1-yn-1-yl]-3-  
pyridinyl]-2-methyl- (CA INDEX NAME)

Double bond geometry as shown.

PAGE 1-A





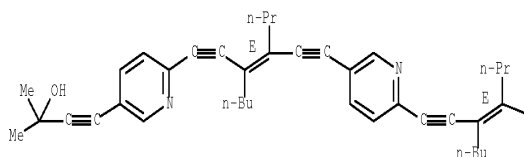


RN 740810-65-5 CAPLUS

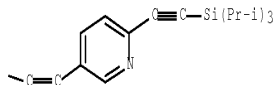
CN 3-Butyn-2-ol, 4-[6-[(3E)-3-butyl-4-[2-[6-[(3E)-3-butyl-4-[2-[6-[2-[tris(1-methylethyl)silyl]ethynyl]-3-pyridinyl]ethynyl]-3-hepten-1-yn-1-yl]-3-pyridinyl]ethynyl]-3-hepten-1-yn-1-yl]-3-pyridinyl]-2-methyl- (CA INDEX NAME)

Double bond geometry as shown.

PAGE 1-A



PAGE 1-B

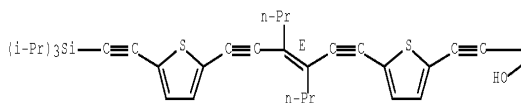


RN 740810-67-7 CAPLUS

CN 3-Butyn-2-ol, 2-methyl-4-[5-[(3E)-3-propyl-4-[5-[tris(1-methylethyl)silyl]ethynyl]-2-thienyl]ethynyl]-3-hepten-1-yn-1-yl]-2-thienyl- (CA INDEX NAME)

Double bond geometry as shown.

PAGE 1-A

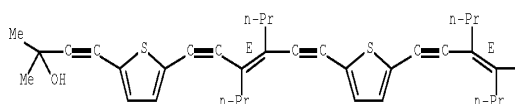


RN 740810-68-8 CAPLUS

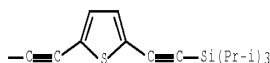
CN 3-Butyn-2-ol, 2-methyl-4-[5-[(3E)-3-propyl-4-[5-[tris(1-methylethyl)silyl]ethynyl]-2-thienyl]ethynyl]-3-hepten-1-yn-1-yl]-2-thienyl- (CA INDEX NAME)

Double bond geometry as shown.

PAGE 1-A



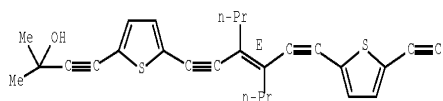
PAGE 1-B



RN 864683-96-5 CAPLUS

CN 3-Butyn-2-ol, 4-[5-[(3E)-5-ethyl-4-[2-(5-ethynyl-2-thienyl)ethynyl]-3-propyl-3-penten-1-yn-1-yl]-2-thienyl]-2-methyl- (CA INDEX NAME)

Double bond geometry as shown.

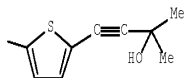
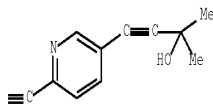
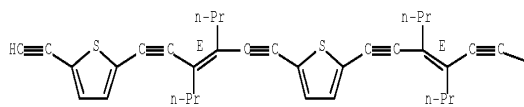


RN 864683-97-6 CAPLUS

CN 3-Butyn-2-ol, 4-[5-[(3E)-4-[2-[5-[(3E)-4-[2-(5-ethynyl-2-thienyl)ethynyl]-3-propyl-3-hepten-1-yn-1-yl]-2-thienyl]ethynyl]-3-propyl-3-hepten-1-yn-1-yl]-2-thienyl]-2-methyl- (CA INDEX NAME)

Double bond geometry as shown.

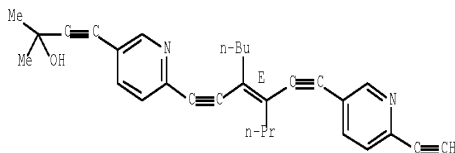




RN 864684-01-5 CAPLUS

CN 3-Butyn-2-ol, 4-[6-[(3E)-3-butyl-4-[2-(6-ethynyl-3-pyridinyl)ethynyl]-3-hepten-1-yn-1-yl]-3-pyridinyl]-2-methyl- (CA INDEX NAME)

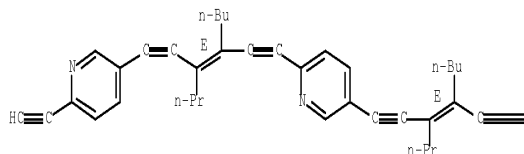
Double bond geometry as shown.



RN 864684-02-6 CAPLUS

CN 3-Butyn-2-ol, 4-[6-[(3E)-3-butyl-4-[2-[6-[(3E)-3-butyl-4-[2-(6-ethynyl-3-pyridinyl)ethynyl]-3-hepten-1-yn-1-yl]-3-pyridinyl]ethynyl]-3-hepten-1-yn-1-yl]-3-pyridinyl]-2-methyl- (CA INDEX NAME)

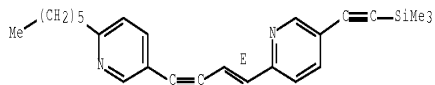
Double bond geometry as shown.



RN 864684-11-7 CAPLUS

CN Pyridine, 2-[(1E)-4-(6-hexyl-3-pyridinyl)-1-buten-3-yn-1-yl]-5-[2-(trimethylsilyl)ethynyl]- (CA INDEX NAME)

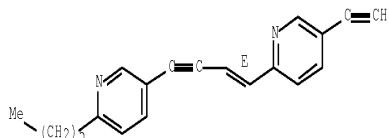
Double bond geometry as shown.



RN 864684-12-8 CAPLUS

CN Pyridine, 5-ethynyl-2-[(1E)-4-(6-hexyl-3-pyridinyl)-1-buten-3-yn-1-yl]- (CA INDEX NAME)

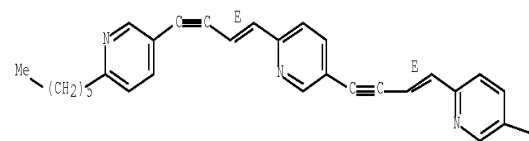
Double bond geometry as shown.



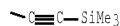
RN 864684-13-9 CAPLUS

CN Pyridine, 2-[(1E)-4-(6-hexyl-3-pyridinyl)-1-buten-3-yn-1-yl]-5-[(3E)-4-[5-[2-(trimethylsilyl)ethynyl]-2-pyridinyl]-3-buten-1-yn-1-yl]- (CA INDEX NAME)

Double bond geometry as shown.



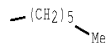
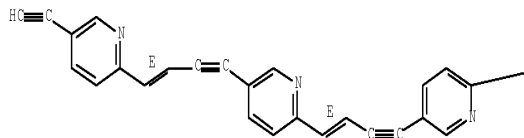




RN 864684-15-1 CAPLUS

CN Pyridine, 5-ethynyl-2-[(1E)-4-[6-[(1E)-4-(6-hexyl-3-pyridinyl)-1-buten-3-yn-1-yl]-3-pyridinyl]-1-buten-3-yn-1-yl]- (CA INDEX NAME)

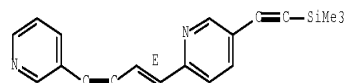
Double bond geometry as shown.



RN 864684-18-4 CAPLUS

CN Pyridine, 2-[(1E)-4-(3-pyridinyl)-1-buten-3-yn-1-yl]-5-[2-(trimethylsilyl)ethynyl]- (CA INDEX NAME)

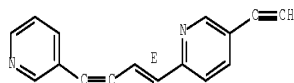
Double bond geometry as shown.



RN 864684-19-5 CAPLUS

CN Pyridine, 5-ethynyl-2-[(1E)-4-(3-pyridinyl)-1-buten-3-yn-1-yl]- (CA INDEX NAME)

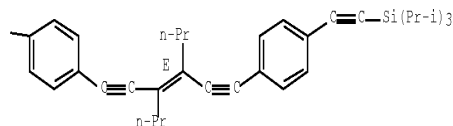
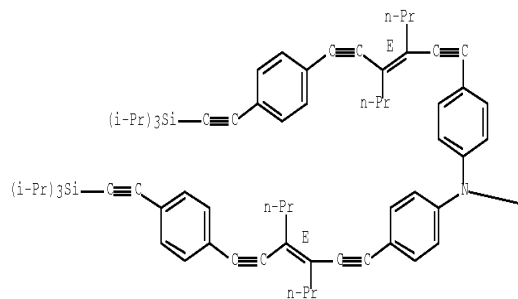
Double bond geometry as shown.



RN 864684-31-1 CAPLUS

CN Benzenamine, N-[4-[(3E)-3,4-dipropyl-6-[4-[2-[tris(1-methylethyl)silyl]ethynyl]phenyl]-3-hexene-1,5-diyn-1-yl]phenyl]-4-[(3E)-3-propyl-4-[2-[4-[2-[tris(1-methylethyl)silyl]ethynyl]phenyl]ethynyl]-3-hepten-1-yn-1-yl]-N-[4-[(3E)-3-propyl-4-[2-[4-[2-[tris(1-methylethyl)silyl]ethynyl]phenyl]ethynyl]-3-hepten-1-yn-1-yl]phenyl]- (CA INDEX NAME)

Double bond geometry as shown.



RN 864684-32-2 CAPLUS

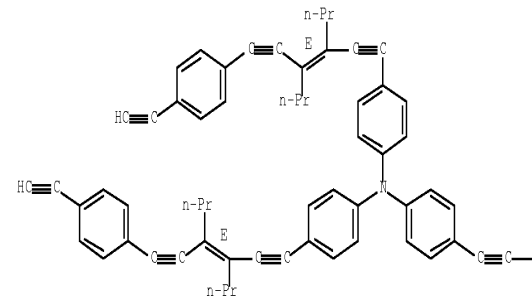
CN Benzenamine, N-[4-[(3E)-5-ethyl-4-[2-(4-ethynylphenyl)ethynyl]-3-propyl-3-



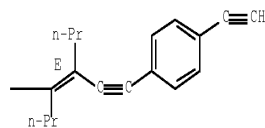
penten-1-yn-1-yl]phenyl]-4-[(3E)-4-[2-(4-ethynylphenyl)ethynyl]-3-propyl-3-hepten-1-yn-1-yl]-N-[4-[(3E)-4-[2-(4-ethynylphenyl)ethynyl]-3-propyl-3-hepten-1-yn-1-yl]phenyl]- (CA INDEX NAME)

Double bond geometry as shown.

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IT	740810-66-6P	740810-63-3P	864684-03-7P
	864684-06-9P	864684-03-3P	864684-16-2P
	864684-17-3P	864684-20-8P	864684-21-5P
	864684-22-0P	864684-23-1P	864684-24-2P
	864684-25-3P	864684-26-4P	864684-27-5P
	864684-28-6P	864684-29-7P	864684-30-0P
	864684-33-3P		

RL: DEV (Device component use); IMF (Industrial manufacture); SPN (Synthetic preparation); TEM (Technical or engineered material use); PREP (Preparation); USES (Uses)

(preparation of  $\pi$ -conjugated aromatic ring-containing acetylene derivs. as organic electroluminescent devices)

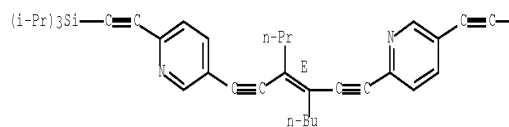
RN 740810-66-6 CAPLUS

CN 3-Butyn-2-ol, 4-[6-[(3E)-3-butyl-4-[2-[6-[(3E)-3-butyl-4-[2-[6-[(3E)-3-

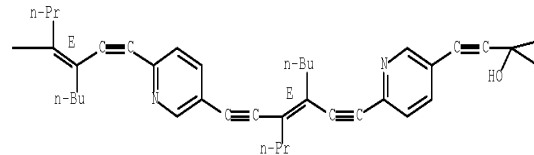
butyl-4-[2-[6-[2-[tris(1-methylethyl)silyl]ethynyl]-3-pyridinyl]ethynyl]-3-hepten-1-yn-1-yl]-3-pyridinyl]ethynyl]-3-hepten-1-yn-1-yl]-3-pyridinyl]ethynyl]-2-methyl- (CA INDEX NAME)

Double bond geometry as shown.

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PAGE 1-B



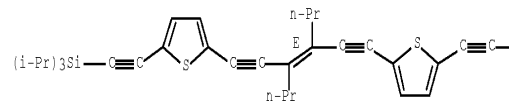
PAGE 1-C



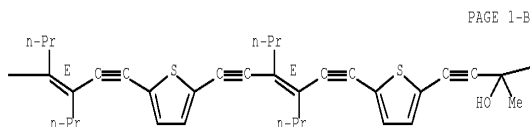
RN 740810-69-9 CAPLUS  
 CN 3-Butyn-2-ol, 4-[5-[(3E)-4-[2-[5-[(3E)-5-ethyl-4-[2-[5-[(3E)-5-ethyl-3-propyl-4-[2-[5-[2-[tris(1-methylethyl)silyl]ethynyl]-2-thienyl]ethynyl]-3-penten-1-yn-1-yl]-2-thienyl]ethynyl]-3-propyl-3-penten-1-yn-1-yl]-2-thienyl]ethynyl]-3-propyl-3-hepten-1-yn-1-yl]-2-thienyl]-2-methyl- (CA INDEX NAME)

Double bond geometry as shown.

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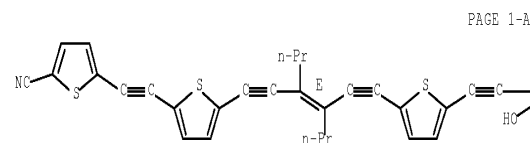


PAGE 1-C



RN 864684-03-7 CAPLUS  
 CN 2-Thiophenecarbonitrile, 5-[2-[5-[(3E)-5-ethyl-4-[2-[5-(3-hydroxy-3-methyl-1-buty-1-yl)-2-thienyl]ethynyl]-3-propyl-3-penten-1-yn-1-yl]-2-thienyl]ethynyl]- (CA INDEX NAME)

Double bond geometry as shown.

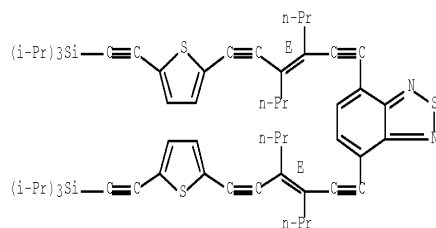


PAGE 1-B



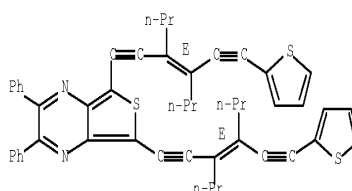
RN 864684-06-0 CAPLUS  
 CN 2,1,3-Benzothiadiazole, 4-[(3E)-3,4-dipropyl-6-[5-[2-[tris(1-methylethyl)silyl]ethynyl]-2-thienyl]-3-hexene-1,5-diyn-1-yl]-7-[(3E)-3-propyl-4-[2-[5-[2-[tris(1-methylethyl)silyl]ethynyl]-2-thienyl]ethynyl]-3-hepten-1-yn-1-yl]- (CA INDEX NAME)

Double bond geometry as shown.



RN 864684-09-3 CAPLUS  
 CN Thieno[3,4-b]pyrazine, 5-[(3E)-3,4-dipropyl-6-(2-thienyl)-3-hexene-1,5-diyn-1-yl]-2,3-diphenyl-7-[(3E)-3-propyl-4-[2-(2-thienyl)ethynyl]-3-hepten-1-yn-1-yl]- (CA INDEX NAME)

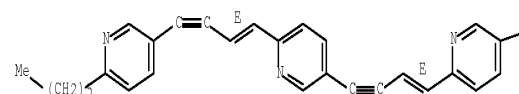
Double bond geometry as shown.



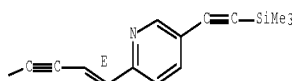
RN 864684-16-2 CAPLUS  
 CN Pyridine, 2-[(1E)-4-[6-[(1E)-4-[6-[(1E)-4-(6-hexyl-3-pyridinyl)-1-buten-3-yn-1-yl]-3-pyridinyl]-1-buten-3-yn-1-yl]-3-pyridinyl]-1-buten-3-yn-1-yl]-5-[2-(trimethylsilyl)ethynyl]- (CA INDEX NAME)

Double bond geometry as shown.

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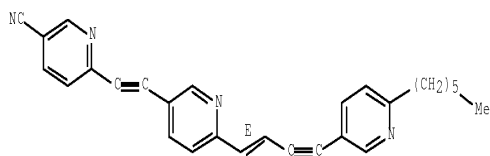
PAGE 1-B





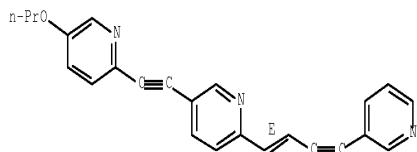
RN 864684-17-3 CAPLUS  
 CN 3-Pyridinecarbonitrile, 6-[2-[6-[(1E)-4-(6-hexyl-3-pyridinyl)-1-buten-3-yn-1-yl]-3-pyridinyl]ethynyl]- (CA INDEX NAME)

Double bond geometry as shown.



RN 864684-20-8 CAPLUS  
 CN Pyridine, 5-[2-(5-propoxy-2-pyridinyl)ethynyl]-2-[(1E)-4-(3-pyridinyl)-1-buten-3-yn-1-yl]- (CA INDEX NAME)

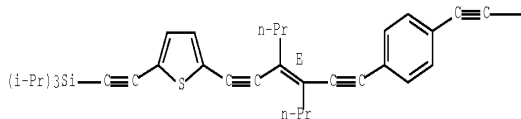
Double bond geometry as shown.



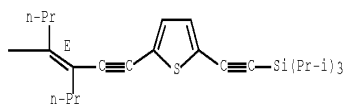
RN 864684-21-9 CAPLUS  
 CN Thiophene, 2-[(3E)-3,4-dipropyl-6-[4-[(3E)-3-propyl-4-[2-[5-[2-[tris(1-methylethyl)silyl]ethynyl]-2-thienyl]ethynyl]-3-hepten-1-yn-1-yl]phenyl]-3-hexene-1,5-diyn-1-yl]-5-[2-[tris(1-methylethyl)silyl]ethynyl]- (CA INDEX NAME)

Double bond geometry as shown.

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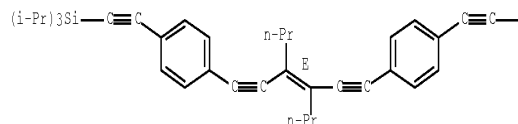
PAGE 1-B



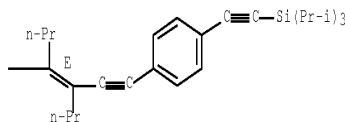
RN 864684-22-0 CAPLUS  
 CN Benzene, 1-[(3E)-3,4-dipropyl-6-[4-[2-[tris(1-methylethyl)silyl]ethynyl]phenyl]-3-hexene-1,5-diyn-1-yl]-4-[(3E)-3-propyl-4-[2-[4-[2-[tris(1-methylethyl)silyl]ethynyl]phenyl]ethynyl]-3-hepten-1-yn-1-yl]- (CA INDEX NAME)

Double bond geometry as shown.

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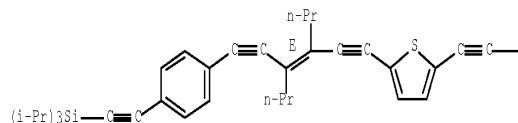
PAGE 1-B



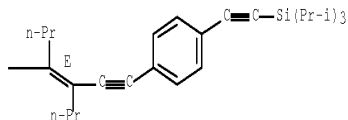
RN 864684-23-1 CAPLUS  
 CN Thiophene, 2-[(3E)-3,4-dipropyl-6-[4-[2-[tris(1-methylethyl)silyl]ethynyl]phenyl]-3-hexene-1,5-diyn-1-yl]-5-[(3E)-3-propyl-4-[2-[4-[2-[tris(1-methylethyl)silyl]ethynyl]phenyl]ethynyl]-3-hepten-1-yn-1-yl]- (CA INDEX NAME)

Double bond geometry as shown.

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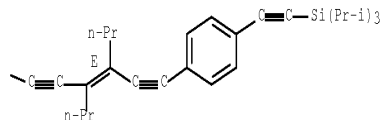




RN 864684-24-2 CAPLUS

CN Silane, [oxybis[4,1-phenylene[(3E)-3,4-dipropyl-3-hexene-1,5-diyne-6,1-diyl]-4,1-phenylene-2,1-ethynediyl]]bis[tris(1-methylethyl)- (9CI) (CA INDEX NAME)

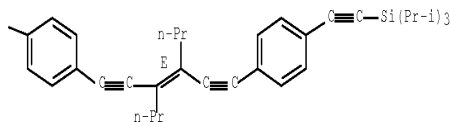
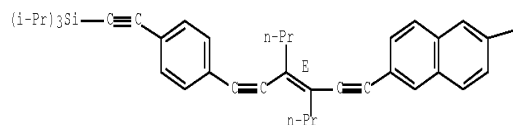
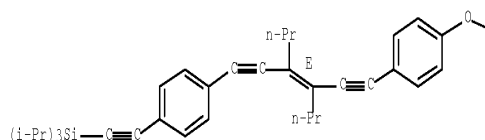
Double bond geometry as shown.



RN 864684-26-4 CAPLUS

CN Naphthalene, 2-[(3E)-3,4-dipropyl-6-[4-[2-[tris(1-methylethyl)silyl]ethynyl]phenyl]-3-hexene-1,5-diyn-1-yl]-6-[(3E)-3-propyl-4-[2-[4-[2-[tris(1-methylethyl)silyl]ethynyl]phenyl]ethynyl]-3-hepten-1-yn-1-yl]- (CA INDEX NAME)

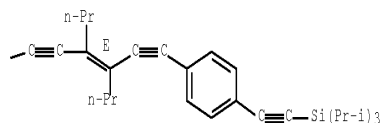
Double bond geometry as shown.



RN 864684-25-3 CAPLUS

CN 2,2'-Bithiophene, 5-[(3E)-3,4-dipropyl-6-[4-[2-[tris(1-methylethyl)silyl]ethynyl]phenyl]-3-hexene-1,5-diyn-1-yl]-5'-[(3E)-3-propyl-4-[2-[4-[2-[tris(1-methylethyl)silyl]ethynyl]phenyl]ethynyl]-3-hepten-1-yn-1-yl]- (CA INDEX NAME)

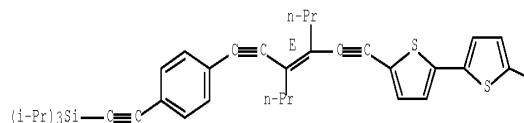
Double bond geometry as shown.



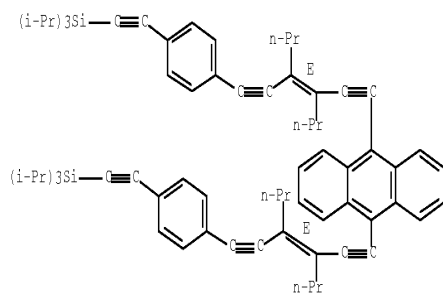
RN 864684-27-5 CAPLUS

CN Anthracene, 9-[(3E)-3,4-dipropyl-6-[4-[2-[tris(1-methylethyl)silyl]ethynyl]phenyl]-3-hexene-1,5-diyn-1-yl]-10-[(3E)-3-propyl-4-[2-[4-[2-[tris(1-methylethyl)silyl]ethynyl]phenyl]ethynyl]-3-hepten-1-yn-1-yl]- (CA INDEX NAME)

Double bond geometry as shown.



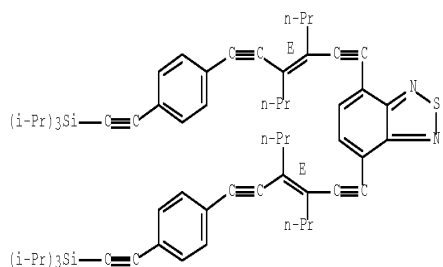




RN 864684-28-6 CAPLUS

CN 2,1,3-Benzothiadiazole, 4-[(3E)-3,4-dipropyl-6-[4-[2-[tris(1-methylethyl)silyl]ethynyl]phenyl]-3-hexene-1,5-diyn-1-yl]-7-[(3E)-3-propyl-4-[2-[4-[2-[tris(1-methylethyl)silyl]ethynyl]phenyl]ethynyl]-3-hepten-1-yn-1-yl]- (CA INDEX NAME)

Double bond geometry as shown.

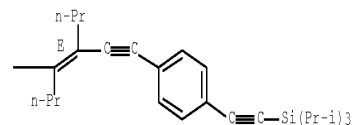
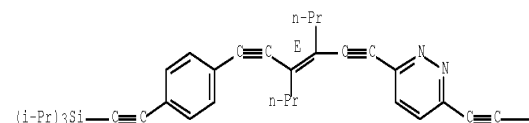


RN 864684-29-7 CAPLUS

CN Pyridazine, 3-[(3E)-3,4-dipropyl-6-[4-[2-[tris(1-methylethyl)silyl]ethynyl]phenyl]-3-hexene-1,5-diyn-1-yl]-6-[(3E)-3-propyl-4-[2-[4-[2-[tris(1-methylethyl)silyl]ethynyl]phenyl]ethynyl]-3-hepten-1-yn-1-yl]- (CA INDEX NAME)

Double bond geometry as shown.

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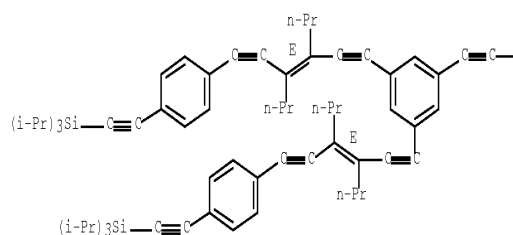


RN 864684-30-0 CAPLUS

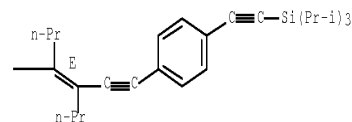
CN Benzene, 1-[(3E)-3,4-dipropyl-6-[4-[2-[tris(1-methylethyl)silyl]ethynyl]phenyl]-3-hexene-1,5-diyn-1-yl]-3-[(3E)-5-ethyl-3-propyl-4-[2-[4-[2-[tris(1-methylethyl)silyl]ethynyl]phenyl]ethynyl]-3-penten-1-yn-1-yl]-5-[(3E)-3-propyl-4-[2-[4-[2-[tris(1-methylethyl)silyl]ethynyl]phenyl]ethynyl]-3-hepten-1-yn-1-yl]- (CA INDEX NAME)

Double bond geometry as shown.

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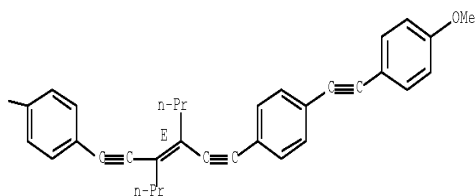
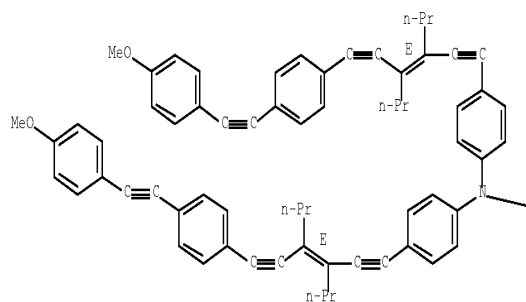


RN 864684-33-3 CAPLUS

CN Benzenamine, N-[4-[(3E)-5-ethyl-4-[2-[4-[2-(4-methoxyphenyl)ethynyl]phenyl]ethynyl]-3-propyl-3-penten-1-yn-1-yl]phenyl]-4-[(3E)-4-[2-[4-[2-(4-methoxyphenyl)ethynyl]phenyl]ethynyl]-3-propyl-3-hepten-1-yn-1-yl]-N-[4-[(3E)-4-[2-[4-[2-(4-methoxyphenyl)ethynyl]phenyl]ethynyl]-3-propyl-3-hepten-1-yn-1-yl]phenyl]- (CA INDEX NAME)

Double bond geometry as shown.

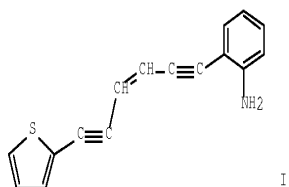




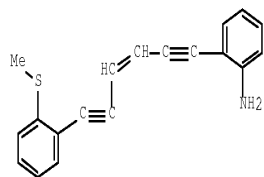
REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L7 ANSWER 10 OF 32 CAPLUS COPYRIGHT 2009 ACS on STN  
 ACCESSION NUMBER: 2005:354187 CAPLUS [Full-text](#)  
 DOCUMENT NUMBER: 143:333  
 TITLE: Cytotoxicities, cell cycle and caspase evaluations of 1,6-diaryl-3(Z)-hexen-1,5-diyne, 2-(6-aryl-3(Z)-hexen-1,5-diynyl)anilines and their derivatives  
 AUTHOR(S): Lin, Chi-Fong; Lo, Yu-Hsiang; Hsieh, Ming-Chu; Chen, Yi-Hua; Wang, Jeh-Jeng; Wu, Ming-Jung  
 CORPORATE SOURCE: School of Chemistry, Kaohsiung Medical University, Kaohsiung, Taiwan  
 SOURCE: Bioorganic & Medicinal Chemistry (2005), 13(10), 3565-3575  
 CODEN: BMECEP; ISSN: 0968-0896  
 PUBLISHER: Elsevier Ltd.  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 OTHER SOURCE(S): CASREACT 143:333

GI



I



II

AB A series of compds. showed growth inhibition effects on a full panel of 60 human cancer cell lines, and most of the average IC50 values of the indicated analogs were from <0.01 to 96.6  $\mu$ M, in which a 2-thienyl analog and the thioanisole analog revealed the highest cytotoxic activity with the cancer cell lines at 10<sup>-7</sup>M concentration range. During the cell cycle anal., a moderate to high apoptotic progress induction was shown by several compared with the control, which 2-(6-(2-thienyl)-3(Z)-hexen-1,5-diynyl)aniline (I) showed the highest apoptotic effect. I and the thioanisole analog displayed a significant G2/M phase arrest in the cell growth cycle compared with other derivs., which the proportions of the G2/M phase cells were accumulated to 71.5% and 82.6%, resp. Moreover, the colorimetric assay of the I and the thioanisole analog also provided advanced evidence to the relationship between the compds. and the caspase-3 enzyme, which was one of the major promoters of apoptotic effect.

IT 852619-13-78

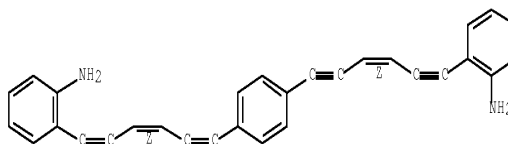
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)

(cytotoxicities, cell cycle and caspase evaluations of 1,6-diaryl-3(Z)-hexen-1,5-diyne, 2-(6-aryl-3(Z)-hexen-1,5-diynyl)anilines and their derivs.)

RN 852619-13-7 CAPLUS

CN Benzenamine, 2,2'-[1,4-phenylenedi-(3Z)-3-hexene-1,5-diyne-6,1-diyl]bis-(9CI) (CA INDEX NAME)

Double bond geometry as shown.





OS.CITING REF COUNT: 15 THERE ARE 15 CAPLUS RECORDS THAT CITE THIS RECORD (15 CITINGS)

REFERENCE COUNT: 35 THERE ARE 35 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L7 ANSWER 11 OF 32 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 2004:832644 CAPLUS Full-text

DOCUMENT NUMBER: 142:38113

TITLE: Site-Selective Monotitanation of Dialkynylpyridines and Its Application for Preparation of Highly

Fluorescent  $\pi$ -Conjugated Oligomers

AUTHOR(S): Takayama, Yuuki; Hanazawa, Takeshi; Andou, Tomohiro; Muraoka, Kenji; Ohtani, Hiroyuki; Takahashi, Mizuki; Sato, Fumie

CORPORATE SOURCE: Department of Biomolecular Engineering, Tokyo Institute of Technology, Midori-ku, Yokohama, Kanagawa, 226-8501, Japan

SOURCE: Organic Letters (2004), 6(23), 4253-4256

CODEN: ORLEF7; ISSN: 1523-7060

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 142:38113

AB Reaction of Ti(O-i-Pr)<sub>4</sub>/2i-PrMgCl reagent with 2,n-bis[(trimethylsilyl)ethynyl]pyridines, where n is 3, 4, 5, and 6, or with 3,4-bis[(trimethylsilyl)ethynyl]pyridines, proceeded with excellent site-selectivity to afford the corresponding monotitanated complex. Synthetic application of the reaction was demonstrated by an efficient preparation of  $\pi$ -conjugated oligomers having pyridine and enyne units alternately, which possess intense blue fluorescence emission. Thus, reaction of 2,3-bis[(trimethylsilyl)ethynyl]pyridine with Ti(O-i-Pr)<sub>4</sub>/2i-PrMgCl reagent in Et<sub>2</sub>O gave 84% (Z)-2-[2-(trimethylsilyl)ethenyl]-3-[(trimethylsilyl)ethynyl]pyridine.

IT 805240-17-9P 805240-18-9P

RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and site-selective monotitanation of dialkynylpyridines and

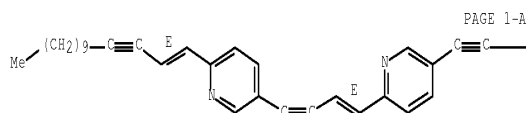
its

application for preparation of highly fluorescent  $\pi$ -conjugated oligomers)

RN 805240-17-9 CAPLUS

CN Pyridine, 2-[(1E)-4-[6-(1E)-1-tetradecen-3-yn-1-yl-3-pyridinyl]-1-buten-3-yn-1-yl]-5-[2-(trimethylsilyl)ethynyl]- (CA INDEX NAME)

Double bond geometry as shown.

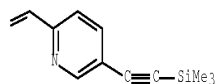
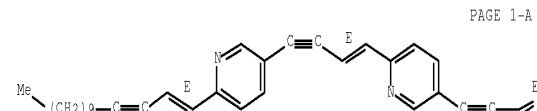


—SiMe<sub>3</sub>

RN 805240-18-0 CAPLUS

CN Pyridine, 2-[(1E)-4-[6-[(1E)-4-[6-(1E)-1-tetradecen-3-yn-1-yl-3-pyridinyl]-1-buten-3-yn-1-yl]-3-pyridinyl]-1-buten-3-yn-1-yl]-5-[2-(trimethylsilyl)ethynyl]- (CA INDEX NAME)

Double bond geometry as shown.



IT 805240-18-1P

RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)

(preparation and site-selective monotitanation of dialkynylpyridines and

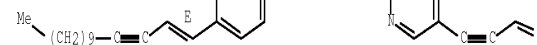
its

application for preparation of highly fluorescent  $\pi$ -conjugated oligomers)

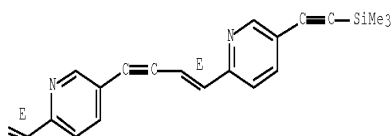
RN 805240-19-1 CAPLUS

CN Pyridine, 2-[(1E)-4-[6-[(1E)-4-[6-[(1E)-4-[6-(1E)-1-tetradecen-3-yn-1-yl-3-pyridinyl]-1-buten-3-yn-1-yl]-3-pyridinyl]-1-buten-3-yn-1-yl]-3-pyridinyl]-1-buten-3-yn-1-yl]-5-[2-(trimethylsilyl)ethynyl]- (CA INDEX NAME)

Double bond geometry as shown.







OS.CITING REF COUNT: 2 THERE ARE 2 CAPLUS RECORDS THAT CITE THIS RECORD (2 CITINGS)

REFERENCE COUNT: 16 THERE ARE 16 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L7 ANSWER 12 OF 32 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 2004:566840 CAPLUS [Full-text](#)

DOCUMENT NUMBER: 141:261152

TITLE:  $\pi$ -Conjugated Dendrimers Based on Bis(enediynyl)benzene Units

AUTHOR(S): Hwang, Gil Tae; Kim, Byeang Hyeon

CORPORATE SOURCE: National Research Laboratory, Department of Chemistry, Division of Molecular and Life Sciences, Pohang University of Science and Technology, Pohang, 790-784, S. Korea

SOURCE: Organic Letters (2004), 6(16), 2669-2672  
CODEN: ORLEF7; ISSN: 1523-7060

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

AB We have synthesized a new family of  $\pi$ -conjugated dendrimers that are based on bis(enediynyl)benzene units by using both divergent and convergent approaches. The compds. at all three generations have strong bluish-green fluorescence, especially the third-generation dendrimer, which has the highest extinction coefficient and quantum efficiency in this series.

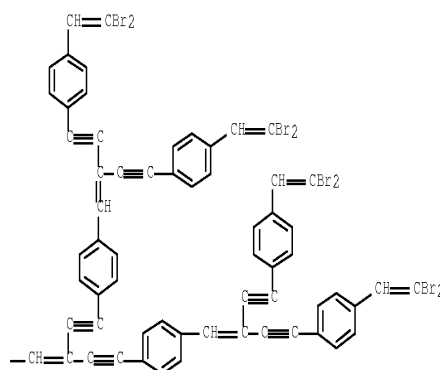
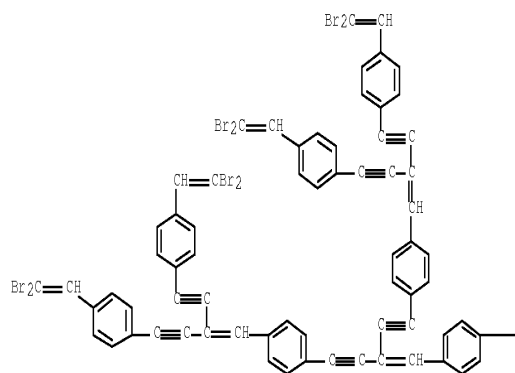
IT 754233-16-4P 754233-18-6P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(convergent and divergent synthesis of  $\pi$ -conjugated dendrimers based on bis(enediynyl)benzene units)

RN 754233-16-4 CAPLUS

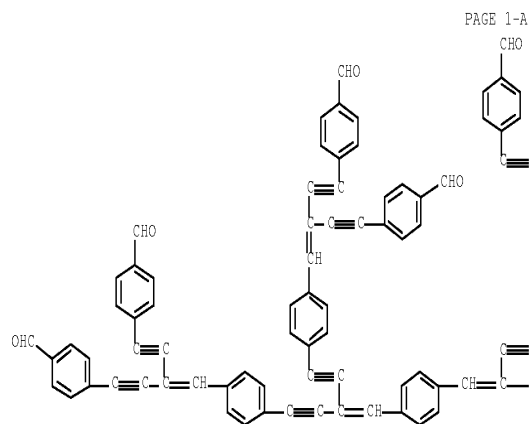
CN Benzene, 1,4-bis[4-[4-[4-(2,2-dibromoethenyl)phenyl]-2-[[4-(2,2-dibromoethenyl)phenyl]ethynyl]-1-buten-3-ynyl]phenyl]-2-[[4-[4-(2,2-dibromoethenyl)phenyl]-2-[[4-(2,2-dibromoethenyl)phenyl]ethynyl]-1-buten-3-ynyl]phenyl]ethynyl]-1-buten-3-ynyl]- (9CI) (CA INDEX NAME)



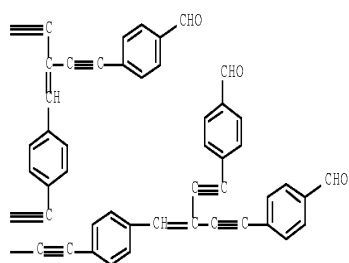
RN 754233-18-6 CAPLUS

CN Benzaldehyde, 4,4'-[[3-[[4-[4-[4-(4-formylphenyl)-2-[(4-formylphenyl)ethynyl]-1-buten-3-ynyl]phenyl]-2-[[4-[4-(4-formylphenyl)-2-[(4-formylphenyl)ethynyl]-1-buten-3-ynyl]phenyl]ethynyl]-1-buten-3-ynyl]phenyl]methylene]-1,4-pentadiyne-1,5-diyl]bis[4,1-phenylene[3-[(4-formylphenyl)ethynyl]-3-buten-1-yne-4,1-diyl]]]bis- (9CI) (CA INDEX NAME)





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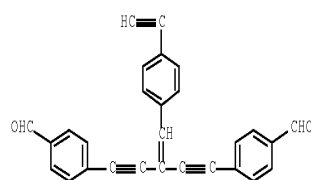


IT 006181-75-1

RL: RCT (Reactant); RACT (Reactant or reagent)  
(in convergent approach; convergent and divergent synthesis of  
 $\pi$ -conjugated dendrimers based on bis(enediynyl)benzene units)

RN 206181-75-1 CAPLUS

CN Benzaldehyde, 4,4'-[3-[(4-ethynylphenyl)methylene]-1,4-pentadiyne-1,5-diyl]bis- (CA INDEX NAME)



OS.CITING REF COUNT: 17 THERE ARE 17 CAPLUS RECORDS THAT CITE THIS  
RECORD (17 CITINGS)  
REFERENCE COUNT: 33 THERE ARE 33 CITED REFERENCES AVAILABLE FOR THIS  
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L7 ANSWER 13 OF 32 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 2004:480115 CAPLUS [Full-text](#)

DOCUMENT NUMBER: 141:190674

TITLE: Synthesis of Conjugated Oligomers Having Aromatic and  
Enediyne Units Alternately in the Backbone that Show  
Intense Fluorescence Emission

AUTHOR(S): Nakano, Yuuki; Ishizuka, Kenichi; Muraoka, Kenji;  
Ohtani, Hiroyuki; Takayama, Yuuki; Sato, Fumie

CORPORATE SOURCE: Department of Biomolecular Engineering, Tokyo  
Institute of Technology, Midori, Yokohama, Kanagawa,  
226-8501, Japan

SOURCE: Organic Letters (2004), 6(14), 2373-2376

CODEN: ORLEF7; ISSN: 1523-7060

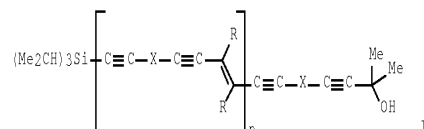
PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 141:190674

GI



AB Synthesis and fluorescence properties of  $\pi$ -conjugated compds. I ( $n = 1 - 3$ ;  $X = 1,4$ -phenylene, 2,5-pyridine, 2,5-thiophene;  $R = n$ -Pr,  $n$ -Bu) having alternately an aromatic or heteroarom. ring and an enediyne unit in the backbone are described.

IT 740610-61-1P 740310-62-2P 740810-64-4P

740310-65-5P 740810-67-7P 740610-68-8P

RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP  
(Preparation); RACT (Reactant or reagent)

(preparation and absorption and fluorescence spectra of conjugated  
oligomers

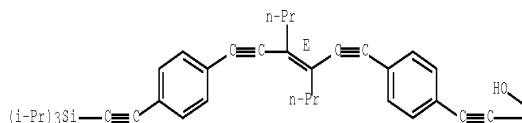
having aromatic (or heteroarom.) and enediyne units alternately in the  
backbone)



RN 740810-61-1 CAPLUS  
 CN 3-Butyn-2-ol, 2-methyl-4-[4-[(3E)-3-propyl-4-[2-[4-[2-[tris(1-methylethyl)silyl]ethynyl]phenyl]ethynyl]-3-hepten-1-yn-1-yl]phenyl]- (CA INDEX NAME)

Double bond geometry as shown.

PAGE 1-A



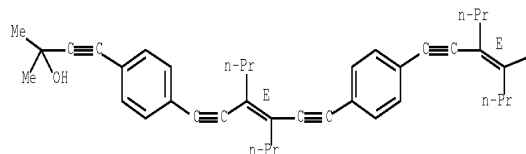
PAGE 1-B



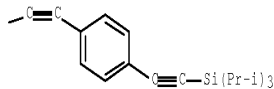
RN 740810-62-2 CAPLUS  
 CN 3-Butyn-2-ol, 2-methyl-4-[4-[(3E)-3-propyl-4-[4-[(3E)-3-propyl-4-[4-[[tris(1-methylethyl)silyl]ethynyl]phenyl]ethynyl]-3-hepten-1-yn-1-yl]phenyl]ethynyl]-3-hepten-1-yn-1-yl]phenyl]- (CA INDEX NAME)

Double bond geometry as shown.

PAGE 1-A



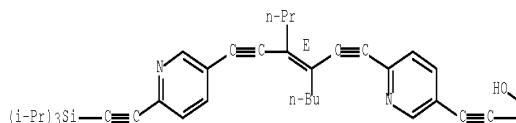
PAGE 1-B



RN 740810-64-4 CAPLUS  
 CN 3-Butyn-2-ol, 4-[6-[(3E)-3-butyl-4-[2-[6-[2-[tris(1-methylethyl)silyl]ethynyl]-3-pyridinyl]ethynyl]-3-hepten-1-yn-1-yl]-3-pyridinyl]-2-methyl- (CA INDEX NAME)

Double bond geometry as shown.

PAGE 1-A



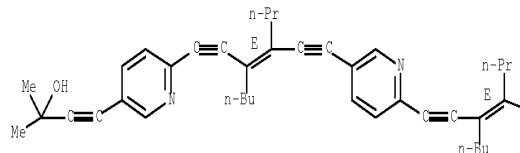
PAGE 1-B



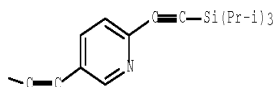
RN 740810-65-5 CAPLUS  
 CN 3-Butyn-2-ol, 4-[6-[(3E)-3-butyl-4-[2-[6-[(3E)-3-butyl-4-[2-[6-[2-[tris(1-methylethyl)silyl]ethynyl]-3-pyridinyl]ethynyl]-3-hepten-1-yn-1-yl]-3-pyridinyl]ethynyl]-3-hepten-1-yn-1-yl]-3-pyridinyl]-2-methyl- (CA INDEX NAME)

Double bond geometry as shown.

PAGE 1-A



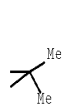
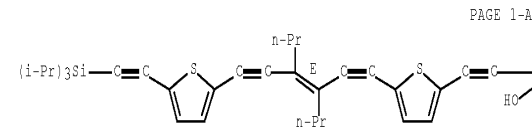
PAGE 1-B





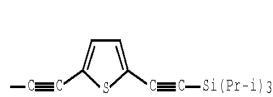
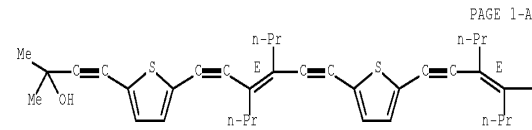
RN 740810-67-7 CAPLUS  
CN 3-Butyn-2-ol, 2-methyl-4-[5-[(3E)-3-propyl-4-[[5-[[tris(1-methylethyl)silyl]ethynyl]-2-thienyl]ethynyl]-3-hepten-1-yn-1-yl]-2-thienyl]- (CA INDEX NAME)

Double bond geometry as shown.



RN 740810-68-8 CAPLUS  
CN 3-Butyn-2-ol, 2-methyl-4-[5-[(3E)-3-propyl-4-[[5-[(3E)-3-propyl-4-[[5-[[tris(1-methylethyl)silyl]ethynyl]-2-thienyl]ethynyl]-3-hepten-1-yn-1-yl]-2-thienyl]ethynyl]-3-hepten-1-yn-1-yl]-2-thienyl]- (CA INDEX NAME)

Double bond geometry as shown.

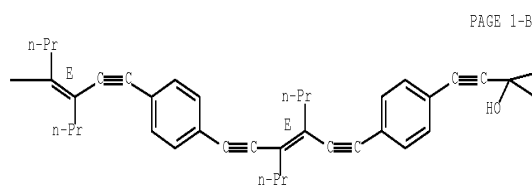
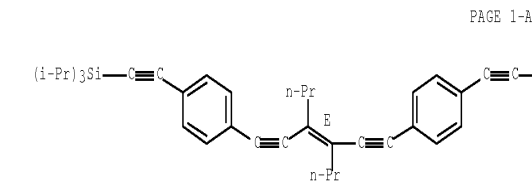


IT 740810-62-3P 740810-66-6P 740810-69-3P  
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)  
(preparation and absorption and fluorescence spectra of conjugated  
oligomers  
having aromatic (or heteroarom.) and enediyne units alternately in the  
backbone)

RN 740810-63-3 CAPLUS  
CN 3-Butyn-2-ol, 2-methyl-4-[4-[(3E)-3-propyl-4-[[4-[(3E)-3-propyl-4-[[4-

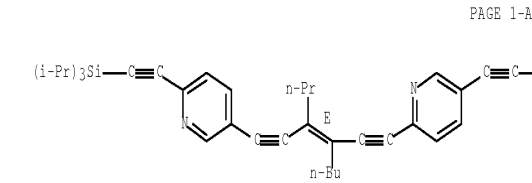
[(3E)-3-propyl-4-[[4-[[tris(1-methylethyl)silyl]ethynyl]phenyl]ethynyl]-3-hepten-1-yn-1-yl]phenyl]ethynyl]-3-hepten-1-yn-1-yl]phenyl]ethynyl]-3-hepten-1-yn-1-yl]phenyl]- (CA INDEX NAME)

Double bond geometry as shown.

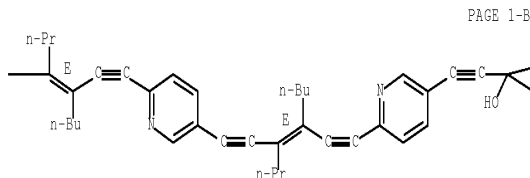


RN 740810-66-6 CAPLUS  
CN 3-Butyn-2-ol, 4-[6-[(3E)-3-butyl-4-[2-[6-[(3E)-3-butyl-4-[2-[6-[(3E)-3-butyl-4-[2-[6-[2-[tris(1-methylethyl)silyl]ethynyl]-3-pyridinyl]ethynyl]-3-hepten-1-yn-1-yl]-3-pyridinyl]ethynyl]-3-hepten-1-yn-1-yl]-3-pyridinyl]ethynyl]-3-hepten-1-yn-1-yl]-3-pyridinyl]ethynyl]-2-methyl- (CA INDEX NAME)

Double bond geometry as shown.







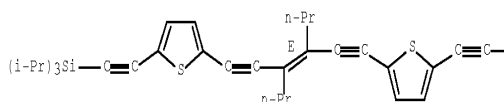
PAGE 1-B



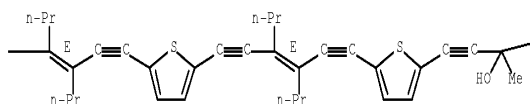
PAGE 1-C

RN 740810-69-9 CAPLUS  
 CN 3-Butyn-2-ol, 4-[5-[(3E)-4-[2-[5-[(3E)-5-ethyl-4-[2-[5-[(3E)-5-ethyl-3-propyl-4-[2-[5-[2-[tris(1-methylethyl)silyl]ethynyl]-2-thienyl]ethynyl]-3-penten-1-yn-1-yl]-2-thienyl]ethynyl]-3-propyl-3-penten-1-yn-1-yl]-2-thienyl]ethynyl]-3-propyl-3-hepten-1-yn-1-yl]-2-thienyl]-2-methyl- (CA INDEX NAME)

Double bond geometry as shown.



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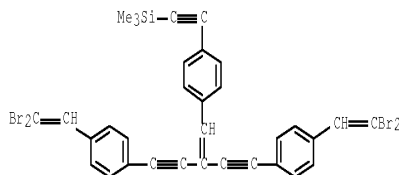
OS.CITING REF COUNT: 20 THERE ARE 20 CAPLUS RECORDS THAT CITE THIS RECORD (20 CITINGS)  
 REFERENCE COUNT: 12 THERE ARE 12 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L7 ANSWER 14 OF 32 CAPLUS COPYRIGHT 2009 ACS on STN  
 ACCESSION NUMBER: 2004:382959 CAPLUS [Full-text](#)  
 DOCUMENT NUMBER: 141:88772  
 TITLE: Electrochemical and theoretical study of a family of fully conjugated dendritic oligomers  
 AUTHOR(S): Osorio, Gabriela; Frontana, Carlos; Guadarrama, Patricia; Frontana-Urbe, Bernardo A.  
 CORPORATE SOURCE: Instituto de Quimica, UNAM, Circuito Exterior Ciudad Universitaria, Mexico, 04510, Mex.  
 SOURCE: Journal of Physical Organic Chemistry (2004), 17(5), 439-447  
 CODEN: JPOCEE; ISSN: 0894-3230  
 PUBLISHER: John Wiley & Sons Ltd.  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English

AB Novel dendritic oligomers of  $\beta,\beta$ -dibromo-4-ethynylstyrene and formyl-4-ethynylstyrene were electrochem. and theor. studied to gain a better insight into their redox behavior. Correlations between calculated ionization and exptl. oxidation potentials (anodic peak potentials) were established. The best correlation was obtained when two important effects are considered in the theor. calcons., probing their strong influence: (a) structural re-accommodation in the formed radical cation and (b) solvation effects. The effect of dendritic terminal groups (dibromovinyl and formyl groups) was also analyzed. A different redox behavior was observed for these two terminal groups, presumably due to a difference in their oxidation mechanisms. A global chemical transformation for the oxidation of dibromovinyl-terminated oligomers was proposed, providing a satisfactory explanation of the electrochem. behavior within this family of (presence of adsorptive phenomena). Taking these results into account, it is possible to explain how the cation-radical species formed in these conjugated dendritic oligomers behave when cyclic voltammetry technique is applied.

IT 716327-89-8 716327-90-1 716327-91-2  
 RL: CPS (Chemical process); FMU (Formation, unclassified); PEP (Physical, engineering or chemical process); PRP (Properties); RCT (Reactant); FORM (Formation, nonpreparative); PROC (Process); RACT (Reactant or reagent) (electrochem. and theor. study of fully conjugated dendritic oligomers family)

RN 716327-89-8 CAPLUS  
 CN Silane, [[4-[4-(2,2-dibromoethenyl)phenyl]-2-[[4-(2,2-dibromoethenyl)phenyl]ethynyl]-1-buten-3-ynyl]phenyl]ethynyl]trimethyl-, radical ion(1+) (9CI) (CA INDEX NAME)

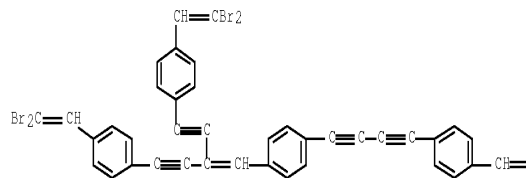




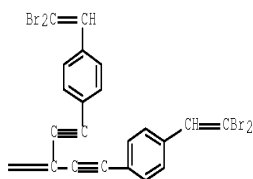
RN 716327-90-1 CAPLUS

CN Benzene, 1,1'-(1,3-butadiyne-1,4-diyl)bis[4-[4-(2,2-dibromoethenyl)phenyl]-2-[[4-(2,2-dibromoethenyl)phenyl]ethynyl]-1-buten-3-ynyl]-, radical ion(1+) (9CI) (CA INDEX NAME)

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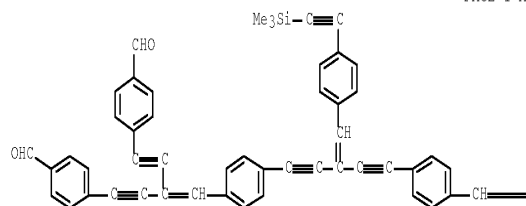
PAGE 1-B



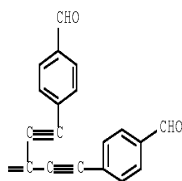
RN 716327-91-2 CAPLUS

CN Benzaldehyde, 4,4'-[[3-[[[4-[(trimethylsilyl)ethynyl]phenyl]methylene]-1,4-pentadiyne-1,5-diyl]bis[4,1-phenylene[3-[(4-formylphenyl)ethynyl]-3-buten-1-yne-4,1-diyl]]]bis-, radical ion(1+) (9CI) (CA INDEX NAME)

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PAGE 1-A



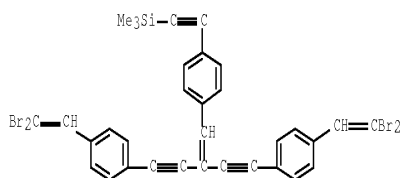
IT 206181-72-8 206181-74-0 206181-76-2

RL: CPS (Chemical process); PEP (Physical, engineering or chemical process); PRP (Properties); RCT (Reactant); PROC (Process); RACT (Reactant or reagent)

(electrochem. and theor. study of fully conjugated dendritic oligomers family)

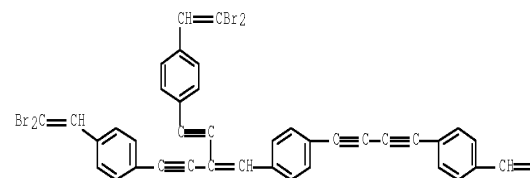
RN 206181-72-8 CAPLUS

CN Silane, [[4-[4-(2,2-dibromoethenyl)phenyl]-2-[[4-(2,2-dibromoethenyl)phenyl]ethynyl]-1-buten-3-ynyl]phenyl]ethynyl]trimethyl- (9CI) (CA INDEX NAME)

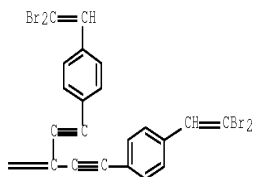


RN 206181-74-0 CAPLUS

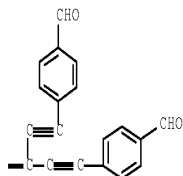
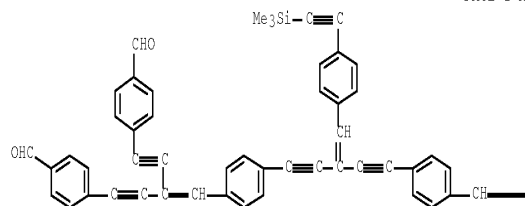
CN Benzene, 1,1'-(1,3-butadiyne-1,4-diyl)bis[4-[4-(2,2-dibromoethenyl)phenyl]-2-[[4-(2,2-dibromoethenyl)phenyl]ethynyl]-1-buten-3-ynyl]- (9CI) (CA INDEX NAME)



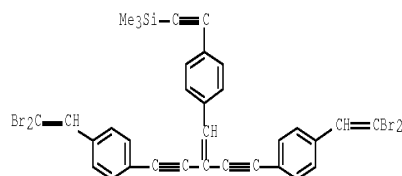




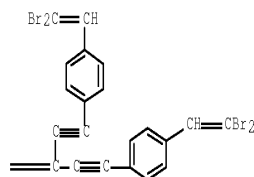
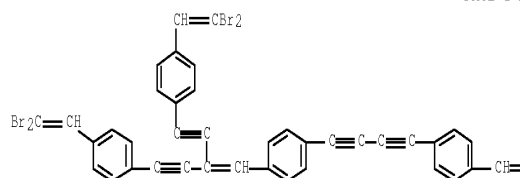
RN 206181-76-2 CAPLUS  
 CN Benzaldehyde, 4,4'-[[3-[[4-[(trimethylsilyl)ethynyl]phenyl]methylene]-1,4-pentadiyne-1,5-diyl]bis[4,1-phenylene[3-[(4-formylphenyl)ethynyl]-3-buten-1-yne-4,1-diyl]]]bis- (9CI) (CA INDEX NAME)



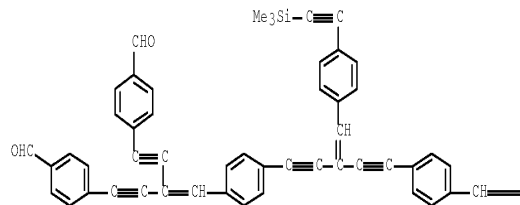
IT 717144-23-5 717144-24-6 717144-25-7  
 RL: FMU (Formation, unclassified); PRP (Properties); RCT (Reactant); FORM (Formation, nonpreparative); RACT (Reactant or reagent)  
 (electrochem. and theor. study of fully conjugated dendritic oligomers family)  
 RN 717144-23-5 CAPLUS  
 CN Silane, [[4-[4-[4-(2,2-dibromoethenyl)phenyl]-2-[[4-(2,2-dibromoethenyl)phenyl]ethynyl]-1-buten-3-ynyl]phenyl]ethynyl]trimethyl-, radical ion(1-) (9CI) (CA INDEX NAME)



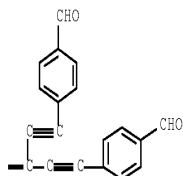
RN 717144-24-6 CAPLUS  
 CN Benzene, 1,1'-(1,3-butadiyne-1,4-diyl)bis[4-[4-(2,2-dibromoethenyl)phenyl]-2-[[4-(2,2-dibromoethenyl)phenyl]ethynyl]-1-buten-3-ynyl]-, radical ion(1-) (9CI) (CA INDEX NAME)



RN 717144-25-7 CAPLUS  
 CN Benzaldehyde, 4,4'-[[3-[[4-[(trimethylsilyl)ethynyl]phenyl]methylene]-1,4-pentadiyne-1,5-diyl]bis[4,1-phenylene[3-[(4-formylphenyl)ethynyl]-3-buten-1-yne-4,1-diyl]]]bis-, radical ion(1-) (9CI) (CA INDEX NAME)







OS.CITING REF COUNT: 2 THERE ARE 2 CAPLUS RECORDS THAT CITE THIS RECORD (2 CITINGS)

REFERENCE COUNT: 31 THERE ARE 31 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L7 ANSWER 15 OF 32 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 2004:328526 CAPLUS [Full-text](#)

DOCUMENT NUMBER: 141:54000

TITLE: Solid-phase synthesis of oligo(triacetylene)s and oligo(phenylenetriacetylene)s employing Sonogashira and Cadiot-Chodkiewicz-type cross-coupling reactions

AUTHOR(S): Utesch, Nils F.; Diederich, Francois; Boudon, Corinne; Gisselbrecht, Jean-Paul; Gross, Maurice

CORPORATE SOURCE: Laboratorium fuer Organische Chemie, ETH-Hoenggerberg, HCI, Zurich, CH-8093, Switz.

SOURCE: Helvetica Chimica Acta (2004), 87(3), 698-718  
CODEN: HCACAV; ISSN: 0018-019X

PUBLISHER: Verlag Helvetica Chimica Acta

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 141:54000

AB The polymer-supported synthesis of poly(triacetylene)-derived monodisperse oligomers is described, using Pd0-catalyzed Sonogashira and Cadiot-Chodkiewicz-type cross-couplings as the key steps in the construction of the acetylenic scaffolds. Merrifield resin functionalized with a 1-(4-iodoaryl)triazene linker was chosen as the polymeric support. The linker selection was made based on the results of several model studies in the liquid phase. For the solid-support synthesis of p-I[C<sub>6</sub>H<sub>4</sub>C.tplbond.CC(CH<sub>2</sub>OSiMe<sub>2</sub>CM<sub>3</sub>):C(CH<sub>2</sub>OSiMe<sub>2</sub>CM<sub>3</sub>)C.tplbond.C]nSiMe<sub>3</sub> (I, n = 2-4) a set of only three reactions was required: (i) Pd0-catalyzed Sonogashira cross-coupling, (ii) Me<sub>3</sub>Si-alkyne deprotection by protodesilylation, and (iii) cleavage of the linker with liberation of I. The longest-wavelength absorption maxima of I [n = 1-4] shift bathochromically with increasing oligomeric length, from λ<sub>max</sub> 337 nm (I, n = 1) to 384 nm (I, n = 4). Based on the electronic absorption data, the effective conjugation length (ECL) of the oligo(phenylene triacetylene)s is estimated to involve at least four monomer units and 40 C-atoms. π-Electron conjugation in these oligomers is less efficient than in Me<sub>3</sub>Si[C<sub>6</sub>H<sub>4</sub>C.tplbond.CC(CH<sub>2</sub>OSiMe<sub>2</sub>CM<sub>3</sub>):C(CH<sub>2</sub>OSiMe<sub>2</sub>CM<sub>3</sub>)C.tplbond.C] nSiMe<sub>3</sub> (II) due to poor transmittance of π-electron delocalization by the Ph rings

inserted into the oligomeric backbone. Similar conclusions were drawn from the electrochem. properties of the two oligomeric series as determined by cyclic (CV) and rotating-disk voltammetry. In sharp contrast to II, I are strongly fluorescent, with the highest quantum yield Φ<sub>F</sub> = 0.69 measured for I [n = 3]. Whereas the Sonogashira cross-coupling on solid support proceeded smoothly, optimal conditions for alkyne-alkyne cross-coupling reactions employing Pd0-catalyzed Cadiot-Chodkiewicz conditions still remain to be developed.

IT 554459-62-0P 554459-63-1P 554459-64-2P

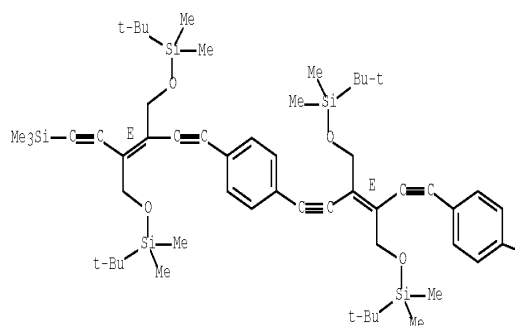
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation) (solid-phase synthesis of oligo(triacetylene)s and oligo(phenylenetriacetylene)s by Sonogashira and Cadiot-Chodkiewicz cross-coupling reactions)

RN 554459-62-0 CAPLUS

CN 4,9-Dioxa-3,10-disiladodec-6-ene, 6-[[4-[(3E)-3,4-bis[[[(1,1-dimethylethyl)dimethylsilyl]oxy]methyl]-6-(4-iodophenyl)-3-hexene-1,5-diynyl]phenyl]ethynyl]-2,2,3,3,10,10,11,11-octamethyl-7-[(trimethylsilyl)ethynyl]-, (6E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

PAGE 1-A



PAGE 1-B

-I

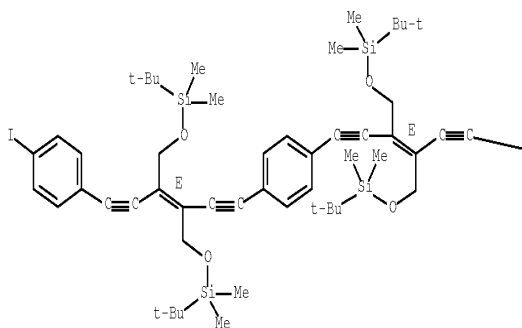
RN 554459-63-1 CAPLUS



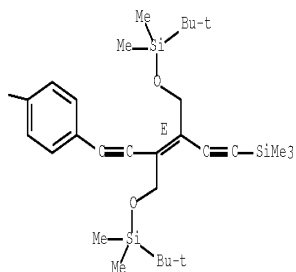
CN 4,9-Dioxa-3,10-disiladodec-6-ene, 6-[[4-[(3E)-6-[4-[(3E)-3,4-bis[[[(1,1-dimethylethyl)dimethylsilyl]oxy]methyl]-6-(4-iodophenyl)-3-hexene-1,5-diynyl]phenyl]-3,4-bis[[[(1,1-dimethylethyl)dimethylsilyl]oxy]methyl]-3-hexene-1,5-diynyl]phenyl]ethynyl]-2,2,3,3,10,10,11,11-octamethyl-7-[(trimethylsilyl)ethynyl]-, (6E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

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PAGE 1-B

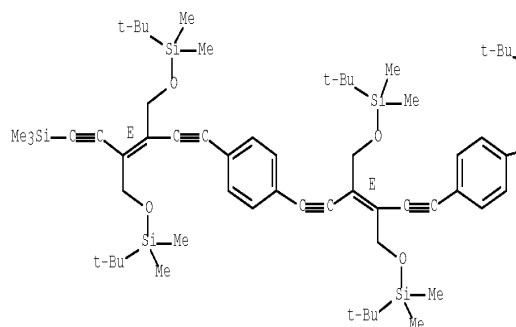


RN 554459-64-2 CAPLUS

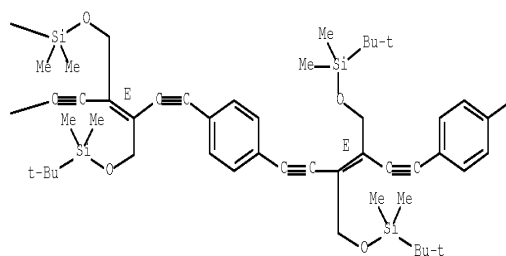
CN 4,9-Dioxa-3,10-disiladodec-6-ene, 6-[[4-[(3E)-6-[4-[(3E)-3,4-bis[[[(1,1-dimethylethyl)dimethylsilyl]oxy]methyl]-6-(4-iodophenyl)-3-hexene-1,5-diynyl]phenyl]-3,4-bis[[[(1,1-dimethylethyl)dimethylsilyl]oxy]methyl]-3-hexene-1,5-diynyl]phenyl]ethynyl]-7-[[4-[(3E)-3,4-bis[[[(1,1-dimethylethyl)dimethylsilyl]oxy]methyl]-6-(trimethylsilyl)-3-hexene-1,5-diynyl]phenyl]ethynyl]-2,2,3,3,10,10,11,11-octamethyl-, (6E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

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PAGE 1-B



IT 704516-23-PP

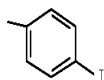
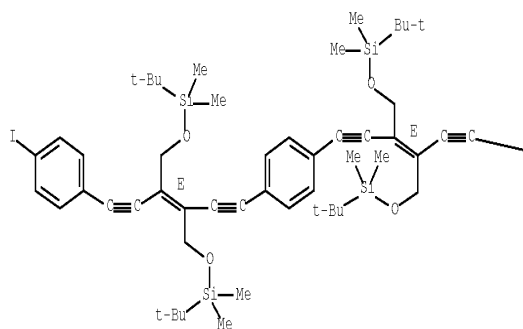
RL: SPN (Synthetic preparation); PREP (Preparation)  
(solid-phase synthesis of oligo(triacetylene)s and  
oligo(phenylenetriacetylene)s by Sonogashira and Cadiot-Chodkiewicz  
cross-coupling reactions)

RN 704916-29-0 CAPLUS

CN 4,9-Dioxa-3,10-disiladodec-6-ene, 6,6'-(1,4-phenylenedi-2,1-ethynediyl)bis[7-[(4-iodophenyl)ethynyl]-2,2,3,3,10,10,11,11-octamethyl-, (6E,6'E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.





OS.CITING REF COUNT: 6 THERE ARE 6 CAPLUS RECORDS THAT CITE THIS RECORD (6 CITINGS)

REFERENCE COUNT: 93 THERE ARE 93 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L7 ANSWER 16 OF 32 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 2003:491916 CAPLUS [Full-text](#)

DOCUMENT NUMBER: 139:395637

TITLE: Synthesis of differentially protected/functionalised acetylenic building blocks from p-benzoquinone and their use in the synthesis of new enediynes

AUTHOR(S): Sankararaman, Sethuraman; Srinivasan, Manivannan

CORPORATE SOURCE: Department of Chemistry, Indian Institute of Technology Madras, Madras, 600 036, India

SOURCE: Organic & Biomolecular Chemistry (2003), 1(13), 2388-2392

CODEN: OBCRAK; ISSN: 1477-0520

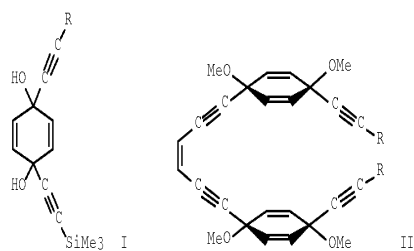
PUBLISHER: Royal Society of Chemistry

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 139:395637

GI



AB Sequential addition of two different lithium acetylides to p-benzoquinone yielded diastereomeric mixts. of 1,4-diethynylcyclohexa-2,5-diene-1,4-diols I [R = (Me<sub>2</sub>CH)<sub>3</sub>Si, (EtO)<sub>2</sub>CH] with different protective/functional groups on the two ethynyl groups. Selective monodeprotection of the di-Me ethers of I to the corresponding terminal acetylenes followed by Pd(0)-mediated coupling with (Z)-1,2-dichloroethene yielded new enediynes II bearing cyclohexa-2,5-diene units.

IT 626235-20-3P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

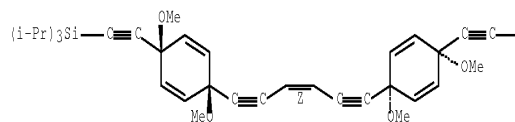
(preparation of cyclohexadienyl enediynes via double addition of functionalized

lithium acetylides to benzoquinone, selective monodeprotection and coupling with dichloroethene)

RN 626235-20-9 CAPLUS

CN Silane, [(3Z)-3-hexene-1,5-diyne-1,6-diylbis[(cis-1,4-dimethoxy-2,5-cyclohexadiene-1,4-diyl)-2,1-ethynediyl]]bis[tris(1-methylethyl)- (9CI) (CA INDEX NAME)

Relative stereochemistry.  
Double bond geometry as shown.



—Si(Pr-i)<sub>3</sub>

IT 626235-21-3P 626235-22-1P

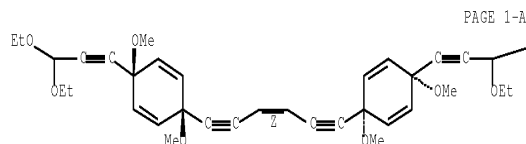
RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation of cyclohexadienyl enediynes via double addition of functionalized



lithium acetylides to benzoquinone, selective monodeprotection and coupling with dichloroethene)  
 RN 626235-21-0 CAPLUS  
 CN 1,4-Cyclohexadiene, 3,3'-(3Z)-3-hexene-1,5-diyne-1,6-diylbis[6-(3,3-diethoxy-1-propynyl)-3,6-dimethoxy-, (cis,cis)- (9CI) (CA INDEX NAME)

Relative stereochemistry.  
 Double bond geometry as shown.



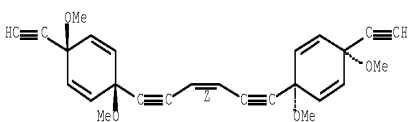
PAGE 1-A

—OEt

PAGE 1-B

RN 626235-22-1 CAPLUS  
 CN 1,4-Cyclohexadiene, 3,3'-(3Z)-3-hexene-1,5-diyne-1,6-diylbis[6-ethynyl-3,6-dimethoxy-, (cis,cis)- (9CI) (CA INDEX NAME)]

Relative stereochemistry.  
 Double bond geometry as shown.

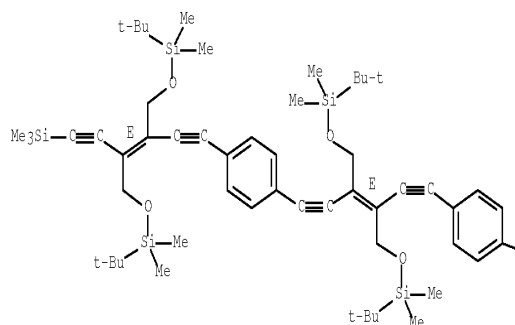


OS.CITING REF COUNT: 6 THERE ARE 6 CAPLUS RECORDS THAT CITE THIS RECORD (6 CITINGS)  
 REFERENCE COUNT: 17 THERE ARE 17 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L7 ANSWER 17 OF 32 CAPLUS COPYRIGHT 2009 ACS on STN  
 ACCESSION NUMBER: 2003:234291 CAPLUS [Full-text](#)  
 DOCUMENT NUMBER: 139:85055  
 TITLE: Acetylenic scaffolding on solid support: Poly(triacetylene)-derived oligomers by Sonogashira and Cadiot-Chodkiewicz-type cross-coupling reactions  
 AUTHOR(S): Utesch, Nils F.; Diederich, Francois  
 CORPORATE SOURCE: Laboratorium fur Organische Chemie, ETH-Honggerberg, HCI, Zurich, CH-8093, Switz.  
 SOURCE: Organic & Biomolecular Chemistry (2003), 1(2), 237-239  
 CODEN: OBCRAK; ISSN: 1477-0520  
 PUBLISHER: Royal Society of Chemistry

DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 OTHER SOURCE(S): CASREACT 139:85055  
 AB Synthesis of poly(triacetylene)-derived oligomers by Pd(0)-catalyzed Sonogashira and Cadiot-Chodkiewicz-type cross-coupling reactions on solid support is reported. Oligo(phenylene triacetylene)s, e.g., I[4-C6H4C.tplbond.CCR:CCR.tplbond.C]nSiMe3 (R = CH2OSiButMe2, n = 1, 2, 3, 4) members of a new class of linearly  $\pi$ -conjugated oligomers with all-C backbones, feature very high fluorescence intensities.  
 IT 554459-62-0P 554459-63-1P 554459-64-2P  
 RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation) (electronic absorption and emission, UV/VIS spectra; poly(triacetylene)-derived oligomers are prepared by Sonogashira and Cadiot-Chodkiewicz-type Pd-catalyzed cross-coupling reactions)  
 RN 554459-62-0 CAPLUS  
 CN 4,9-Dioxa-3,10-disiladodec-6-ene, 6-[[4-[(3E)-3,4-bis[[[(1,1-dimethylethyl)dimethylsilyl]oxy]methyl]-6-(4-iodophenyl)-3-hexene-1,5-diynyl]phenyl]ethynyl]-2,2,3,3,10,10,11,11-octamethyl-7-[(trimethylsilyl)ethynyl]-, (6E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



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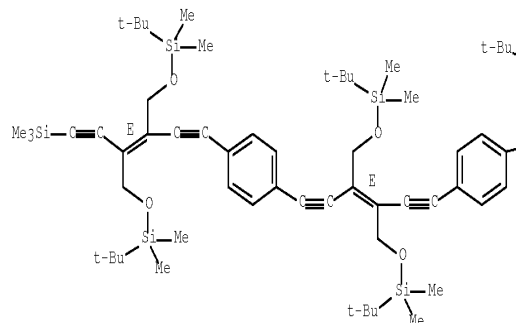
—I



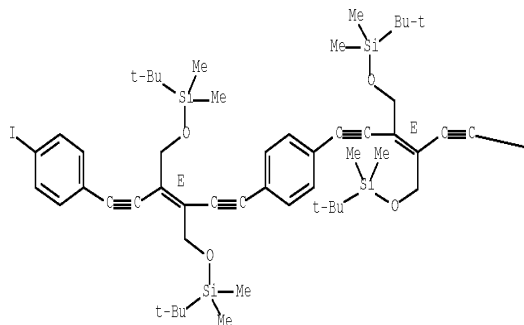
RN 554459-63-1 CAPLUS  
 CN 4,9-Dioxa-3,10-disiladodec-6-ene, 6-[[4-[(3E)-6-[4-[(3E)-3,4-bis[[[(1,1-dimethylethyl)dimethylsilyl]oxy]methyl]-6-(4-iodophenyl)-3-hexene-1,5-diynyl]phenyl]-3,4-bis[[[(1,1-dimethylethyl)dimethylsilyl]oxy]methyl]-3-hexene-1,5-diynyl]phenyl]ethynyl]-2,2,3,3,10,10,11,11-octamethyl-7-[(trimethylsilyl)ethynyl]-, (6E)- (9CI) (CA INDEX NAME)

PAGE 1-A

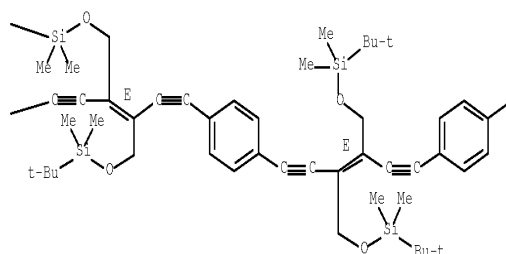
Double bond geometry as shown.



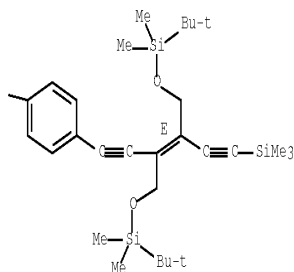
PAGE 1-A



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PAGE 1-B



IT 554459-71-1DE, Merrifield resin-supported  
 554459-72-2DE, Merrifield resin-supported 554459-73-3DE  
 , Merrifield resin-supported  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT  
 (Reactant or reagent)  
 (preparation and Sonogashira and Cadiot-Chodkiewicz-type Pd-catalyzed  
 cross-coupling reactions of supported poly(triacetylene)-derived  
 oligomers)

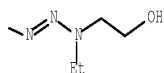
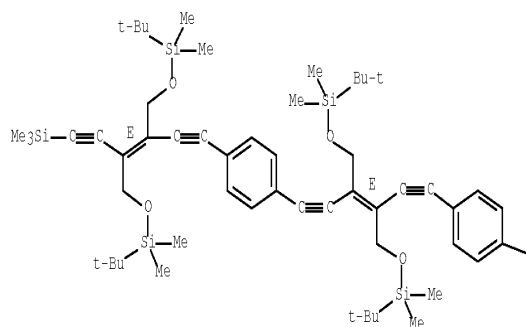
RN 554459-64-2 CAPLUS  
 CN 4,9-Dioxa-3,10-disiladodec-6-ene, 6-[[4-[(3E)-6-[4-[(3E)-3,4-bis[[[(1,1-dimethylethyl)dimethylsilyl]oxy]methyl]-6-(4-iodophenyl)-3-hexene-1,5-diynyl]phenyl]-3,4-bis[[[(1,1-dimethylethyl)dimethylsilyl]oxy]methyl]-3-hexene-1,5-diynyl]phenyl]ethynyl]-7-[[4-[(3E)-3,4-bis[[[(1,1-dimethylethyl)dimethylsilyl]oxy]methyl]-6-(trimethylsilyl)-3-hexene-1,5-diynyl]phenyl]ethynyl]-2,2,3,3,10,10,11,11-octamethyl-, (6E)- (9CI) (CA INDEX NAME)

RN 554459-71-1 CAPLUS  
 CN Ethanol, 2-[3-[4-[(3E)-6-[4-[(3E)-3,4-bis[[[(1,1-dimethylethyl)dimethylsilyl]oxy]methyl]-6-(trimethylsilyl)-3-hexene-1,5-diyn-1-yl]phenyl]-3,4-bis[[[(1,1-dimethylethyl)dimethylsilyl]oxy]methyl]-3-hexene-1,5-diyn-1-yl]phenyl]-1-ethyl-2-triazene-1-yl]- (CA INDEX NAME)

Double bond geometry as described by E or Z.

Double bond geometry as shown.

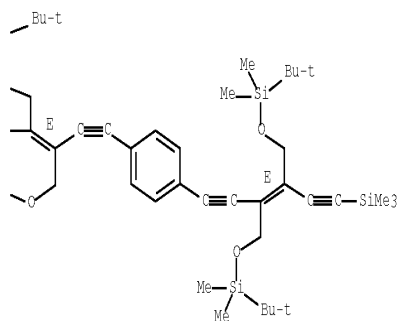
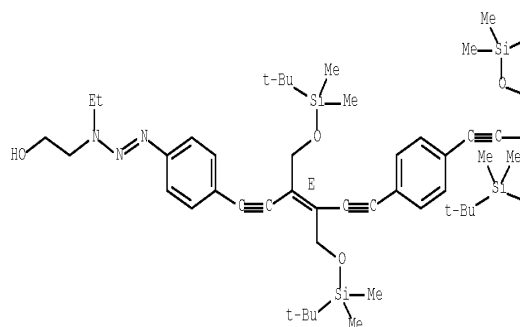




RN 554459-72-2 CAPLUS

CN Ethanol, 2-[3-[4-[(3E)-6-[4-[(3E)-6-[4-[(3E)-3,4-bis[[[(1,1-dimethylethyl)dimethylsilyl]oxy]methyl]-6-(trimethylsilyl)-3-hexene-1,5-diyn-1-yl]phenyl]-3,4-bis[[[(1,1-dimethylethyl)dimethylsilyl]oxy]methyl]-3-hexene-1,5-diyn-1-yl]phenyl]-3,4-bis[[[(1,1-dimethylethyl)dimethylsilyl]oxy]methyl]-3-hexene-1,5-diyn-1-yl]phenyl]-1-ethyl-2-triazene-1-yl]- (CA INDEX NAME)

Double bond geometry as described by E or Z.



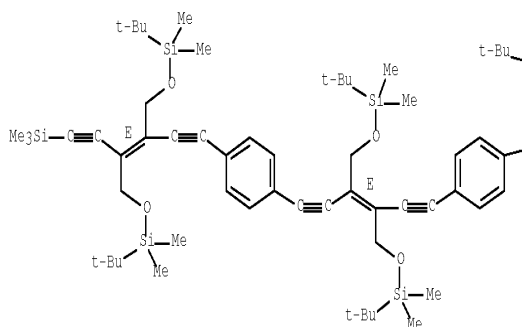
RN 554459-73-3 CAPLUS

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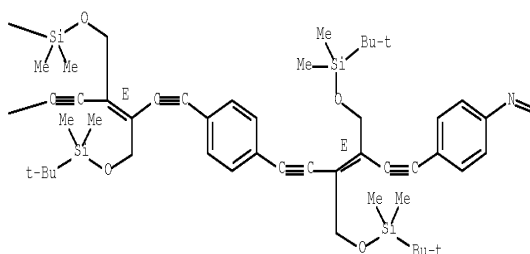
Double bond geometry as described by E or Z.



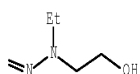
DOCUMENT NUMBER: 137:208374  
TITLE: Manufacturing method of semiconductor device using  
mask pattern having high etching resistance  
INVENTOR(S): Chuchi, Junko; Sato, Yasuhiko; Shiobara, Eishi;  
Hayashi, Hisataka; Ohiwa, Tokuhisa; Onishi, Yasunobu  
PATENT ASSIGNEE(S): Kabushiki Kaisha Toshiba, Japan  
SOURCE: U.S. Pat. Appl. Publ., 26 pp.  
CODEN: USXXCO  
DOCUMENT TYPE: Patent  
LANGUAGE: English  
FAMILY ACC. NUM. COUNT: 1  
PATENT INFORMATION:



PAGE 1-B



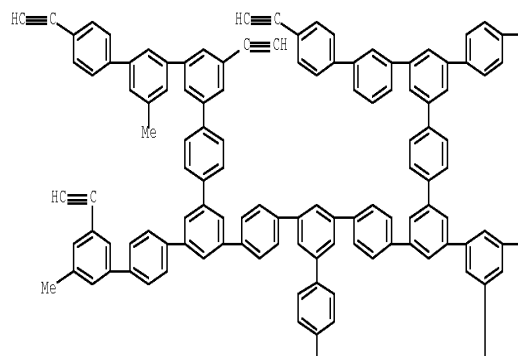
PAGE 1-C



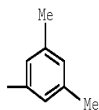
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REFERENCE COUNT:	38	THERE ARE 38 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L7 ANSWER 18 OF 32 CAPLUS COPYRIGHT 2009 ACS on STN  
ACCESSION NUMBER: 2002:658690 CAPLUS Full-text

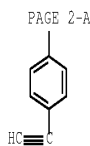
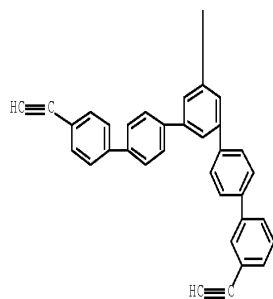
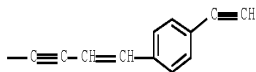
PAGE 1-A







PAGE 1-B



PAGE 2-A

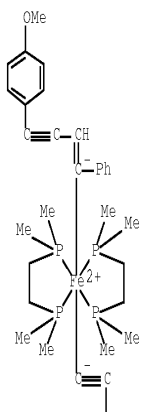
OS.CITING REF COUNT: 8 THERE ARE 8 CAPLUS RECORDS THAT CITE THIS RECORD  
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L7 ANSWER 19 OF 32 CAPLUS COPYRIGHT 2009 ACS on STN  
ACCESSION NUMBER: 2002:198497 CAPLUS [Full-text](#)  
DOCUMENT NUMBER: 136:401857  
TITLE: Acetylide-Bridged Organometallic Oligomers via the  
Photochemical Metathesis of Methyl-Iron(II) Complexes  
AUTHOR(S): Field, Leslie D.; Turnbull, Anthony J.; Turner, Peter  
CORPORATE SOURCE: School of Chemistry, The University of Sydney, Sydney,  
2006, Australia  
SOURCE: Journal of the American Chemical Society (2002),  
124(14), 3692-3702  
CODEN: JACSAT; ISSN: 0002-7863  
PUBLISHER: American Chemical Society  
DOCUMENT TYPE: Journal  
LANGUAGE: English  
OTHER SOURCE(S): CASREACT 136:401857

AB The acetylide Me iron(II) complexes, cis/trans-[Fe(dmpe)<sub>2</sub>(C.tplbond.CR)(CH<sub>3</sub>)] (1) and trans-[Fe(depe)<sub>2</sub>(C.tplbond.CR)(CH<sub>3</sub>)] (2) (dmpe = 1,2-dimethylphosphinoethane; depe = 1,2-diethylphosphinoethane), were synthesized by transmetalation from the corresponding alkyl halide complexes. Acetylide Me iron(II) complexes were also formed by transmetalation from the chloride complexes, trans-[Fe(dmpe)<sub>2</sub>(C.tplbond.CR)(Cl)] or trans-[Fe(depe)<sub>2</sub>(C.tplbond.CR)(Cl)]. The structure of trans-[Fe(dmpe)<sub>2</sub>(C.tplbond.CC6H5)(CH<sub>3</sub>)] (1a) was determined by single-crystal x-ray diffraction. The Me acetylide iron complexes, [Fe(dmpe)<sub>2</sub>(C.tplbond.CR)(CH<sub>3</sub>)] (1), are thermally stable in the presence of acetylenes; however, under UV irradiation, methane is lost with the formation of a metal bisacetylide. Photochem. metathesis of cis- or trans-[Fe(dmpe)<sub>2</sub>(CH<sub>3</sub>)(C.tplbond.CR)] (R = C<sub>6</sub>H<sub>5</sub> (1a), 4-C<sub>6</sub>H<sub>4</sub>OCH<sub>3</sub> (1b)) with terminal acetylenes was used to selectively synthesize unsym. substituted iron(II) bisacetylide complexes of the type trans-[Fe(dmpe)<sub>2</sub>(C.tplbond.CR)(C.tplbond.CR')] [R = Ph, R' = Ph (6a), 4-CH<sub>3</sub>OC<sub>6</sub>H<sub>4</sub> (6b), tBu (6c), SiMe<sub>3</sub> (6d), (CH<sub>2</sub>)<sub>4</sub>C.tplbond.CH (6e); R = 4-CH<sub>3</sub>OC<sub>6</sub>H<sub>4</sub>, R' = 4-CH<sub>3</sub>OC<sub>6</sub>H<sub>4</sub>, (6g), tBu (6h), (CH<sub>2</sub>)<sub>4</sub>C.tplbond.CH (6i), adamantyl (6j)]. The structure of the unsym. iron(II) bisacetylide complex trans-[Fe(dmpe)<sub>2</sub>(C.tplbond.CC6H5)(C.tplbond.CC6H4OCH<sub>3</sub>)] (6b) was determined by single-crystal x-ray diffraction. The photochem. metathesis of the bisacetylene, 1,7-octadiyne, with trans-[Fe(dmpe)<sub>2</sub>(CH<sub>3</sub>)(C.tplbond.CPh)] (1a), was utilized to synthesize the bridged binuclear species trans,trans-[(C<sub>6</sub>H<sub>5</sub>C.tplbond.C)Fe(dmpe)<sub>2</sub>(μ-C.tplbond.C(CH<sub>2</sub>)<sub>4</sub>C.tplbond.C)Fe(dmpe)<sub>2</sub>(C.tplbond.CC6H5)] (11). The trinuclear species trans,trans,trans-[(C<sub>6</sub>H<sub>5</sub>C.tplbond.C)Fe(dmpe)<sub>2</sub>(μ-C.tplbond.C(CH<sub>2</sub>)<sub>4</sub>C.tplbond.C)Fe(dmpe)<sub>2</sub>(μ-C.tplbond.C(CH<sub>2</sub>)<sub>4</sub>C.tplbond.C)Fe(dmpe)<sub>2</sub>(C.tplbond.CC6H5)] (12) was synthesized by the photochem. reaction of Fe(dmpe)<sub>2</sub>(C.tplbond.CPh)(C.tplbond.C(CH<sub>2</sub>)<sub>4</sub>C.tplbond.CH) (6e) with Fe(dmpe)<sub>2</sub>(CH<sub>3</sub>)<sub>2</sub>. Extended irradiation of the bisacetylide complexes with phenylacetylene resulted in insertion of the terminal alkyne into one of the metal acetylide bonds to give acetylide butenyne complexes. The structure of the acetylide butenyne complex, trans-[Fe(dmpe)<sub>2</sub>(C.tplbond.CC6H4OCH<sub>3</sub>)(η<sup>1</sup>-C(C<sub>6</sub>H<sub>5</sub>):CH(C.tplbond.CC6H4OCH<sub>3</sub>))] (9a) was determined by single-crystal x-ray diffraction.

IT 425380-70-78  
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)  
(preparation and crystal structure of)  
RN 425380-70-7 CAPLUS  
CN Iron, bis[1,2-ethanediylbis(dimethylphosphine-κP)][(4-methoxyphenyl)ethynyl][(1E)-4-(4-methoxyphenyl)-1-phenyl-1-buten-3-ynyl]-, (OC-6-11)- (9CI) (CA INDEX NAME)





OS.CITING REF COUNT: 13 THERE ARE 13 CAPLUS RECORDS THAT CITE THIS RECORD (13 CITINGS)

REFERENCE COUNT: 72 THERE ARE 72 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L7 ANSWER 20 OF 32 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 2001:714296 CAPLUS [Full-text](#)

DOCUMENT NUMBER: 136:69640

TITLE: Synthesis and spectroscopic studies of expanded planar dehydrotribenzo[n]annulenes containing one or two isolated alkene units

AUTHOR(S): Wan, W. Brad; Chiechi, Ryan C.; Weakley, Timothy J. R.; Haley, Michael M.

CORPORATE SOURCE: Department of Chemistry and the Materials Science Institute, University of Oregon, Eugene, OR, 97403-1253, USA

SOURCE: European Journal of Organic Chemistry (2001), (18), 3485-3490

CODEN: EJOCFK; ISSN: 1434-193X

PUBLISHER: Wiley-VCH Verlag GmbH

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 136:69640

GI

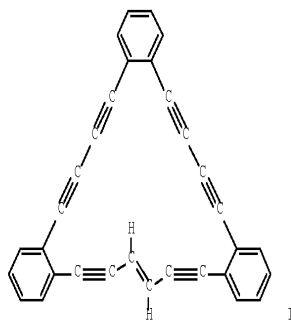
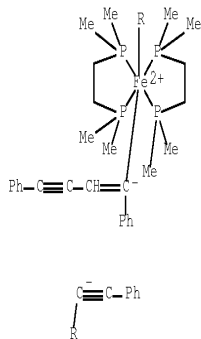


IT 425380-85-4P

RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of)

RN 425380-85-4 CAPLUS

CN Iron, [(1E)-1,4-diphenyl-1-buten-3-ynyl]bis[1,2-ethanediy]bis(dimethylphosphine-κP)] (phenylethynyl)-, (OC-6-11)-(9CI) (CA INDEX NAME)



AB Dehydrobenzoannulene derivs. containing isolated alkene linkages, e.g., I, were synthesized by combining an in situ Pd/Cu-mediated cross-coupling with an intramol. cyclization strategy. 1H NMR studies of these macrocycles and comparison with related systems verify that highly alkynylated dehydrobenzoannulenes possess weak induced ring currents, indicative of aromatic (4n+2 π systems) and antiarom. (4n π systems) behavior, in spite of their large size and extensive benzannulation.

IT 214628-17-4P 214628-18-4P 383404-36-4P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)



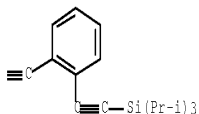
(preparation and spectroscopic studies of expanded planar dehydrotribenzo[n]annulenes containing one or two isolated alkene units)

RN 214628-17-8 CAPLUS

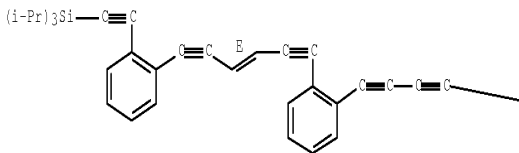
CN Silane, tris(1-methylethyl)[[2-[(3E)-6-[2-[4-[2-[[tris(1-methylethyl)silyl]ethynyl]phenyl]-1,3-butadiynyl]phenyl]-3-hexene-1,5-diynyl]phenyl]ethynyl]- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

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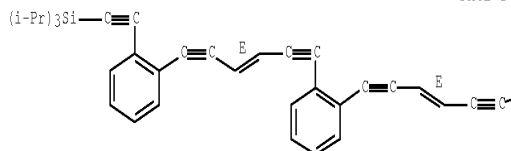


RN 383404-38-4 CAPLUS

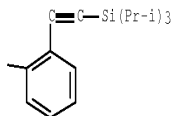
CN Silane, [1,2-phenylenebis[(3E)-3-hexene-1,5-diyne-6,1-diyl-2,1-phenylene-2,1-ethynediyl]]bis[tris(1-methylethyl)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

PAGE 1-A



PAGE 1-B

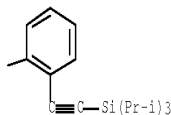


PAGE 1-B

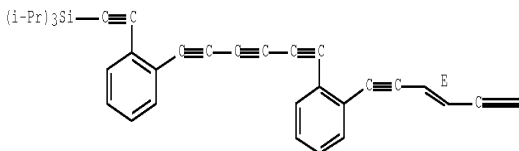
RN 214628-18-9 CAPLUS

CN Silane, tris(1-methylethyl)[[2-[6-[2-[(3E)-6-[2-[[tris(1-methylethyl)silyl]ethynyl]phenyl]-3-hexene-1,5-diynyl]phenyl]-1,3,5-hexatriynyl]phenyl]ethynyl]- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



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OS.CITING REF COUNT: 10 THERE ARE 10 CAPLUS RECORDS THAT CITE THIS RECORD (10 CITINGS)

REFERENCE COUNT: 33 THERE ARE 33 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L7 ANSWER 21 OF 32 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 2000:832492 CAPLUS [Full-text](#)

DOCUMENT NUMBER: 134:310920

TITLE: Bis(enediynes) Macrocycles: Synthesis, Reactivity, and Structural Analysis

AUTHOR(S): Blanchette, H. S.; Brand, S. C.; Naruse, H.; Weakley, T. J. R.; Haley, M. M.

CORPORATE SOURCE: Department of Chemistry, University of Oregon, Eugene, OR, 97403-1253, USA

SOURCE: Tetrahedron (2000), 56(49), 9581-9588

CODEN: TETRAB; ISSN: 0040-4020

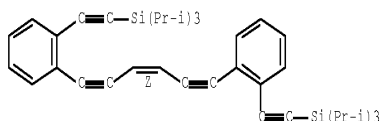
PUBLISHER: Elsevier Science Ltd.

DOCUMENT TYPE: Journal



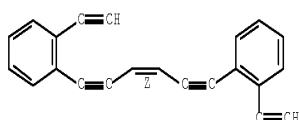
LANGUAGE: English  
 OTHER SOURCE(S): CASREACT 134:310920  
 AB The authors describe the syntheses of five macrocycles possessing two enediyne warheads, along with the structural and thermal analyses of these bis(enediyne) compds. The solid-state packing of one of the compds. suggests the possibility for the mol. to undergo a topochem. diacetylene polymerization  
 IT 335378-20-8P 335378-30-8P  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
 (preparation of bis(enediyne) macrocycles)  
 RN 335378-20-6 CAPLUS  
 CN Silane, [(3Z)-3-hexene-1,5-diyne-1,6-diylbis(2,1-phenylene-2,1-ethynediyl)]bis[tris(1-methylethyl)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



RN 335378-30-8 CAPLUS  
 CN Benzene, 1,1'-[(3Z)-3-hexene-1,5-diyne-1,6-diylbis(2-ethynyl)- (9CI) (CA INDEX NAME)

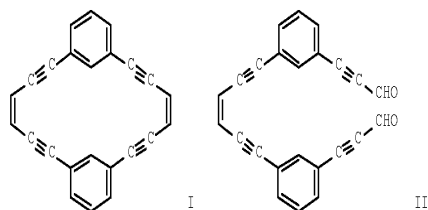
Double bond geometry as shown.



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L7 ANSWER 22 OF 32 CAPLUS COPYRIGHT 2009 ACS on STN  
 ACCESSION NUMBER: 2000:767122 CAPLUS Full-text  
 DOCUMENT NUMBER: 134:71381  
 TITLE: Synthesis and structure of a new [6.6]metacyclophane with enediyne bridges  
 AUTHOR(S): Srinivasan, Manivannan; Sankararaman, Sethuraman; Dix, Ina; Jones, Peter G.  
 CORPORATE SOURCE: Department of Chemistry, Indian Institute of Technology, Madras, 600 036, India  
 SOURCE: Organic Letters (2000), 2(24), 3849-3851  
 CODEN: ORLEF7; ISSN: 1523-7060  
 PUBLISHER: American Chemical Society  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English

OTHER SOURCE(S): CASREACT 134:71381  
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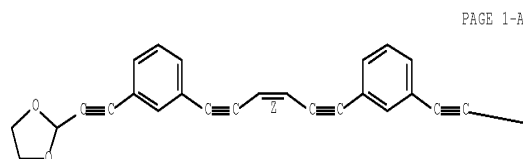


AB Synthesis and structure of a novel [6.6]metacyclophane with enediyne bridges I is reported. I was prepared by reacting 1,3-diethynylbenzene with EtMgBr/THF and DMF to give the monoaldehyde. The monoaldehyde was subsequently converted to the acetal, coupled with ClCH:CHCl to give bis-acetal, which was hydrolyzed to the dialdehyde II. II underwent McMurry coupling using TiCl3 and Zn-Cu couple in DME to give I in 69% yield.

IT 315716-90-6P 315716-91-7P  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
 (preparation and crystal structure of metacyclophane with enediyne bridges)

RN 315716-90-6 CAPLUS  
 CN 1,3-Dioxolane, 2,2'-[(3Z)-3-hexene-1,5-diyne-1,6-diylbis(3,1-phenylene-2,1-ethynediyl)]bis- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



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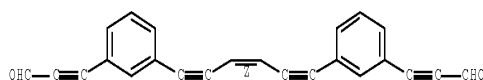


PAGE 1-B

RN 315716-91-7 CAPLUS  
 CN 2-Propynal, 3,3'-[(3Z)-3-hexene-1,5-diyne-1,6-diylbis(3,1-phenylene)]bis- (9CI) (CA INDEX NAME)

Double bond geometry as shown.





OS.CITING REF COUNT: 18 THERE ARE 18 CAPLUS RECORDS THAT CITE THIS RECORD (18 CITINGS)

REFERENCE COUNT: 31 THERE ARE 31 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L7 ANSWER 23 OF 32 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1999:673316 CAPLUS [Full-text](#)

DOCUMENT NUMBER: 131:337589

TITLE: Electronic structure of fully conjugated dendritic oligomers of  $\beta,\beta$ -dibromo-4-ethynyl styrene

AUTHOR(S): Fomine, Sergei; Fomina, Lioudmila; Guadarrama, Patricia

CORPORATE SOURCE: Universidad Nacional Autonoma Mexico, Inst de Investigaciones en Materiales, Coyoacan, 04510 CU, Mex.

SOURCE: THEOCHEM (1999), 488, 207-216  
CODEN: THEODJ; ISSN: 0166-1280

PUBLISHER: Elsevier Science B.V.

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Quantum-mech. calcons. of fully conjugated dendritic oligomers carried out at B3LYP/3-21G//HF/3-21G (d) and B3LYP/3-21G//PM3 levels of theory showed that loose dendritic architecture of  $\beta,\beta$ -dibromo-4-ethynyl styrene oligomers contributes little to the instability and conjugation disruption compared to 1  $\rightarrow$  2 branched polyacetylene, while Br terminal atoms in dendrimers strongly affect the electronic d. distribution in studied mols. On the one hand the bulky bromine atoms decrease the conjugation in Br-terminated dendrimers caused by steric hindrances, on the other hand, highly polarizable bromine atoms reduced significantly adiabatic ionization potentials (IPa) to be up to 1.5 eV lower than corresponding vertical potentials (IPv). Another phenomenon contributing to the reducing of IPa's of all dendrimers is the flattening of mol. geometry accompanying the ionization thus allowing better delocalization of pos. charge over the conjugated system while all aromatic ring except the very outer layer lost their aromaticity becoming essentially quinone by nature.

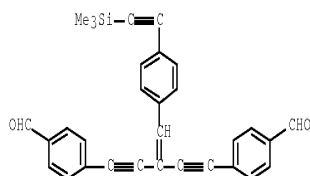
IT 206181-71-7 206181-72-8 206181-73-9  
206181-74-0 206181-75-1 206181-76-2  
206181-77-3 206181-78-4 206181-79-5

RL: PRP (Properties)

(electronic structure of fully conjugated dendritic oligomers of  $\beta,\beta$ -dibromo-4-ethynyl styrene)

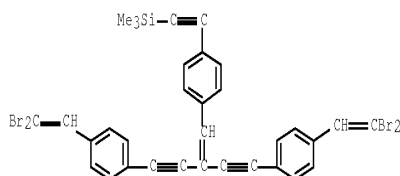
RN 206181-71-7 CAPLUS

CN Benzaldehyde, 4,4'-[3-[[4-[(trimethylsilyl)ethynyl]phenyl]methylene]-1,4-pentadiyne-1,5-diyl]bis- (9CI) (CA INDEX NAME)



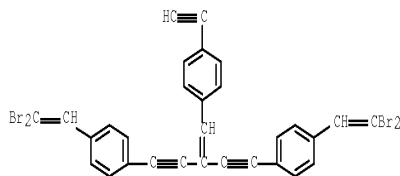
RN 206181-72-8 CAPLUS

CN Silane, [[4-[4-(2,2-dibromoethenyl)phenyl]-2-[[4-(2,2-dibromoethenyl)phenyl]ethynyl]-1-buten-3-ynyl]phenyl]ethynyl]trimethyl- (9CI) (CA INDEX NAME)



RN 206181-73-9 CAPLUS

CN Benzene, 1,1'-[3-[(4-ethynylphenyl)methylene]-1,4-pentadiyne-1,5-diyl]bis[4-(2,2-dibromoethenyl)- (9CI) (CA INDEX NAME)

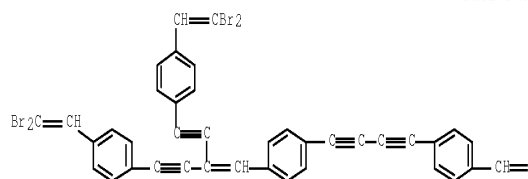


RN 206181-74-0 CAPLUS

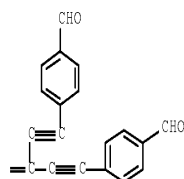
CN Benzene, 1,1'-(1,3-butadiyne-1,4-diyl)bis[4-[4-(2,2-dibromoethenyl)phenyl]-2-[[4-(2,2-dibromoethenyl)phenyl]ethynyl]-1-buten-3-ynyl]- (9CI) (CA INDEX NAME)



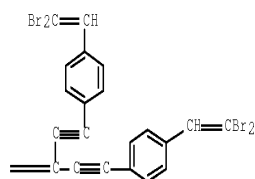
PAGE 1-A



PAGE 1-B

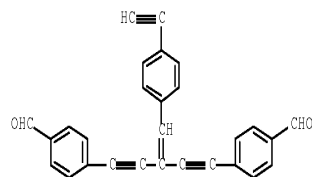


PAGE 1-B

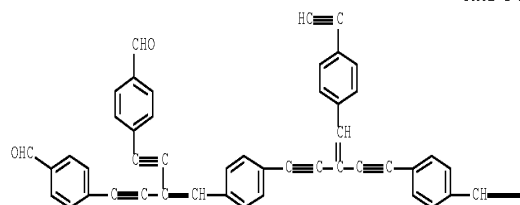


RN 206181-77-3 CAPLUS  
CN Benzaldehyde, 4,4'-[[3-[(4-ethynylphenyl)methylene]-1,4-pentadiyne-1,5-diyl]bis[4,1-phenylene[3-[(4-formylphenyl)ethynyl]-3-buten-1-yne-4,1-diyl]]bis- (9CI) (CA INDEX NAME)

RN 206181-75-1 CAPLUS  
CN Benzaldehyde, 4,4'-[[3-[(4-ethynylphenyl)methylene]-1,4-pentadiyne-1,5-diyl]bis- (CA INDEX NAME)



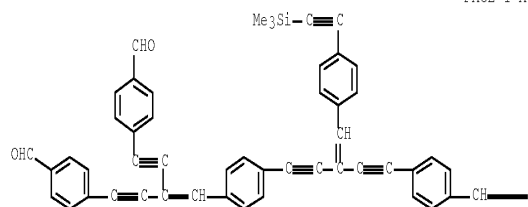
PAGE 1-A



PAGE 1-B

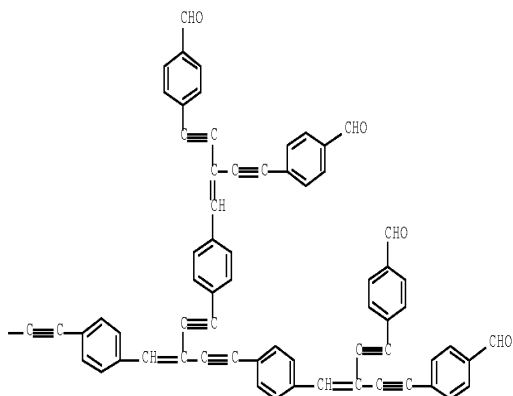
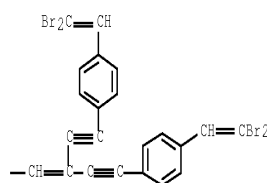
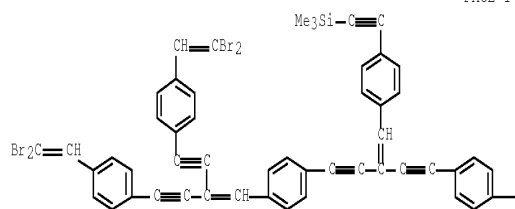
RN 206181-76-2 CAPLUS  
CN Benzaldehyde, 4,4'-[[3-[[4-[(trimethylsilyl)ethynyl]phenyl]methylene]-1,4-pentadiyne-1,5-diyl]bis[4,1-phenylene[3-[(4-formylphenyl)ethynyl]-3-buten-1-yne-4,1-diyl]]bis- (9CI) (CA INDEX NAME)

PAGE 1-A



RN 206181-78-4 CAPLUS  
CN Benzaldehyde, 4,4'-[1,3-butadiyne-1,4-diylbis[4,1-phenylene[3-[[4-[(4-formylphenyl)-2-[(4-formylphenyl)ethynyl]-1-buten-3-ynyl]phenyl]ethynyl]-3-buten-1-yne-4,1-diyl]-4,1-phenylene[3-[(4-formylphenyl)ethynyl]-3-buten-1-yne-4,1-diyl]]bis- (9CI) (CA INDEX NAME)





OS.CITING REF COUNT: 2 THERE ARE 2 CAPLUS RECORDS THAT CITE THIS RECORD  
(2 CITINGS)  
REFERENCE COUNT: 16 THERE ARE 16 CITED REFERENCES AVAILABLE FOR THIS  
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L7 ANSWER 24 OF 32 CAPLUS COPYRIGHT 2009 ACS ON STN

ACCESSION NUMBER: 1999:650836 CAPLUS [Full-text](#)

DOCUMENT NUMBER: 132:16702

TITLE: Theoretical description of luminescent effects in  
 $\beta,\beta$ -di(4'-formylphenylethynyl)-4-  
ethynylstyrene

AUTHOR(S): Salcedo, R.; Guadarrama, P.; Sansores, L. E.; Fomine,  
S.; Fomina, L.

CORPORATE SOURCE: Inst. de Investigaciones en Materiales, Inst. de  
Investigaciones en Materiales, UNAM, Mexico, 04510,  
Mex.

SOURCE: Materials Research Society Symposium Proceedings  
(1999), 560(Luminescent Materials), 359-364  
CODEN: MRSPDH; ISSN: 0272-9172

PUBLISHER: Materials Research Society

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Theor. calcons. at HF/6-31 G(d) level were carried out on fully conjugated  
compds. (4-ethynylbenzaldehyde,  $\beta,\beta$ -dibromo-4-ethynylstyrene,  $\beta,\beta$ -Di(4'-  
formylphenylethynyl)-4-ethynylstyrene and its dimmer) to understand the source  
of blue emission observed in oligomers of the 1st and 2nd generation in CHCl<sub>3</sub>  
solns. The frontier orbitals are distributed through the framework of the  
mols. (benzene rings, double and triple bonds and chromophores). Addnl., a CI  
approach was applied over  $\beta,\beta$ -Di(4'-formylphenylethynyl)-4-ethynylstyrene

RN 206181-79-5 CAPLUS

CN Silane, [[4-[4-[4-[4-(2,2-dibromoethenyl)phenyl]-2-[[4-(2,2-  
dibromoethenyl)phenyl]ethynyl]-1-buten-3-ynyl]phenyl]-2-[[4-[4-[4-(2,2-  
dibromoethenyl)phenyl]-2-[[4-(2,2-dibromoethenyl)phenyl]ethynyl]-1-buten-3-  
ynyl]phenyl]ethynyl]-1-buten-3-ynyl]phenyl]ethynyl]trimethyl- (9CI) (CA  
INDEX NAME)



(compound 3) at CIS/6-31 G(d) level to modeling excited states and simulate the UV-visible spectrum exptl. obtained. Calculated transitions corresponded to S0→S1 which are, presumably, responsible for the fluorescence observed

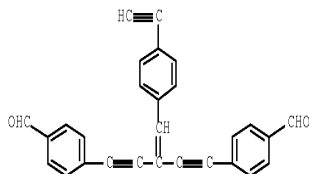
IT 206181-75-1 251479-84-2

RL: PEP (Physical, engineering or chemical process); PRP (Properties); PROC (Process)

(theor. description of luminescent effects in styrene derivs.)

RN 206181-75-1 CAPLUS

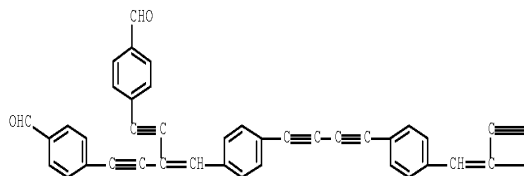
CN Benzaldehyde, 4,4'-[3-[(4-ethynylphenyl)methylene]-1,4-pentadiyne-1,5-diyl]bis- (CA INDEX NAME)



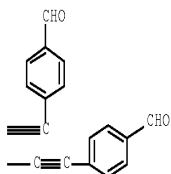
RN 251479-84-2 CAPLUS

CN Benzaldehyde, 4,4'-[1,3-butadiyne-1,4-diylbis[4,1-phenylene[3-[(4-formylphenyl)ethynyl]-3-buten-1-yne-4,1-diyl]]]bis- (9CI) (CA INDEX NAME)

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PAGE 1-B



OS.CITING REF COUNT: 1 THERE ARE 1 CAPLUS RECORDS THAT CITE THIS RECORD (1 CITINGS)

REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L7 ANSWER 25 OF 32 CAPLUS COPYRIGHT 2009 ACS ON STN

ACCESSION NUMBER: 1998:756297 CAPLUS Full-text

DOCUMENT NUMBER: 130:118607

TITLE: Porphyrin-[(E)-1,2-diethynylethene] scaffolding. Synthesis and optical and electrochemical properties of multinanometer-sized porphyrin arrays

AUTHOR(S): Wytko, Jennifer; Berl, Volker; McLaughlin, Mark; Tykwinski, Rik R.; Schreiber, Martin; Diederich, Francois; Boudon, Corinne; Gisselbrecht, Jean-Paul; Gross, Maurice

CORPORATE SOURCE: Laboratorium Organische Chemie, ETH-Zentrum, Zurich, CH-8092, Switz.

SOURCE: Helvetica Chimica Acta (1998), 81(11), 1964-1977

CODEN: HCACAV; ISSN: 0018-019X

PUBLISHER: Verlag Helvetica Chimica Acta AG

DOCUMENT TYPE: Journal

LANGUAGE: English

GI

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

AB Two series of linearly conjugated hybrid materials, consisting of (E)-1,2-diethynylethene (DEE; hex-3-ene-1,5-diyne) and Zn(II) porphyrin components, were prepared by Pd0-catalyzed cross-coupling reactions. In 1 series, 1 or 2 DEE substituents were introduced into the meso-positions of the Zn(II) porphyrins, leading from Zn 5,15-bis{[(ethoxycarbonyl)propoxy]phenyl}porphinate (1) to I and II (n = 1; R = SiMe2tBu). The second series contains the linearly  $\pi$ -conjugated mol. rods III (n = 1-3) that span a length range from 23 Å for III (n = 1) to 53 Å for III (n = 3). The larger rods III (n = 2 and 3) consist of 2 or 3 porphyrin moieties, resp., that are bridged at the meso-positions by trans-enediynediyl (hex-3-ene-1,5-diyne-1,6-diyl) linkers. The UV/VIS spectra in the series I, II, and III (n = 1) showed a strong bathochromic shift of both Soret and Q bands of the Zn(II) porphyrin as a result of the addition of DEE substituents. Upon changing from I to II, the Q band was further bathochromically shifted, whereas the Soret band remained nearly at the same position but became broadened and displayed a shoulder on the lower-wavelength edge as a result of excitonic coupling. The close resemblance between the UV/Vis spectra of III (n = 2 and 3) suggests that saturation of the optical properties in the oligomeric series already occurs at the stage of dimeric III (n = 2). Stationary voltammetric investigations showed that the DEE substituents act as strong electron acceptors which induce large anodic shifts in the 1st reduction potential upon changing from I to II ( $\Delta E$  = 190 mV) and to III (n = 1) ( $\Delta E$  = 340 mV). Increasing the number of porphyrin moieties upon changing from III (n = 1) to III (n = 2) had no effect on the 1st reduction potential yet the 1st oxidation potential was substantially lowered ( $\Delta E$  = 110 mV). Large differences in the potentials for 1-electron oxidation of the 2 porphyrin moieties in III (n = 2) ( $\Delta E$  = 200 mV) confirmed the existence of substantial electronic communication between the 2 macrocycles across the trans-enediynediyl bridge.

IT 213483-19-9

RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

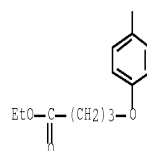
(preparation, UV spectra, electrochem. redox behavior and conversion to trinuclear complex and NMR)

RN 219483-19-9 CAPLUS

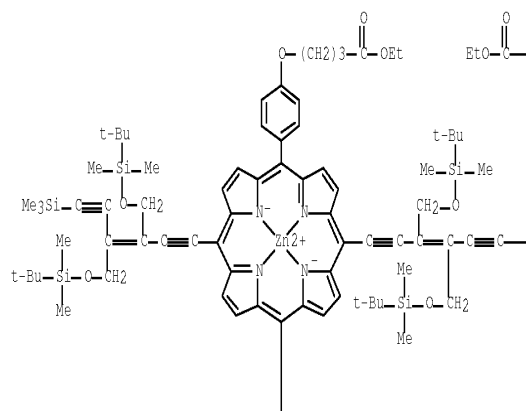


CN Zinc, [ $\mu$ -[[tetraethyl 4,4',4'',4'''-[[[(3E)-3,4-bis[[[(1,1-dimethylethyl)dimethylsilyl]oxy]methyl]-3-hexene-1,5-diyne-1,6-diyl]bis[[20-[(3E)-3,4-bis[[[(1,1-dimethylethyl)dimethylsilyl]oxy]methyl]-6-(trimethylsilyl)-3-hexene-1,5-diyne]]-21H,23H-porphine-10,5,15-triyl- $\kappa$ N21, $\kappa$ N22, $\kappa$ N23, $\kappa$ N24]-4,1-phenyleneoxy]]tetrakis[butanoato]](4-)]di- (9CI) (CA INDEX NAME)

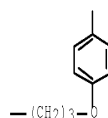
PAGE 2-A



PAGE 1-A



PAGE 2-B



OS.CITING REF COUNT: 45 THERE ARE 45 CAPLUS RECORDS THAT CITE THIS RECORD (45 CITINGS)  
REFERENCE COUNT: 64 THERE ARE 64 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L7 ANSWER 26 OF 32 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1998:606810 CAPLUS [Full-text](#)

DOCUMENT NUMBER: 129:302407

ORIGINAL REFERENCE NO.: 129:61683a,61686a

TITLE: Synthesis of expanded planar dehydrobenzoannulenes: weakly diatropic, weakly paratropic, or atropic?

AUTHOR(S): Wan, W. Brad; Kimball, David B.; Haley, Michael M.

CORPORATE SOURCE: Department of Chemistry, University of Oregon, Oregon, 97403-1253, USA

SOURCE: Tetrahedron Letters (1998), 39(38), 6795-6798

CODEN: TELEAY; ISSN: 0040-4039

PUBLISHER: Elsevier Science Ltd.

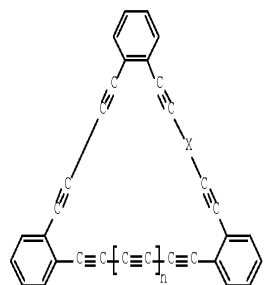
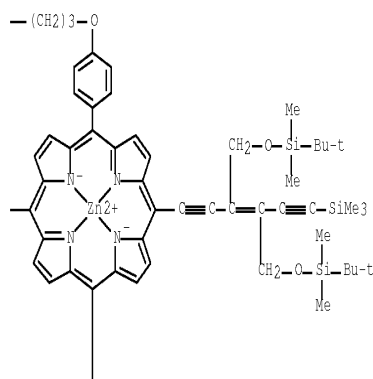
DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 129:302407

GI

PAGE 1-B





AB Use of a Cu/Pd cross-coupling strategy has led to the synthesis of the first dehydrobenzoannulenes I [X = C.tplbond.C, (E)-CH:CH; n = 0,1] containing triacetylenic linkages. NMR studies of these macrocycles and comparison with other known systems indicate that, in spite of their large size and extensive benzannulation, dehydrobenzoannulenes possess weak induced ring currents.

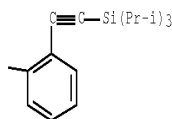
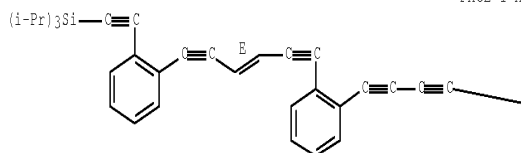
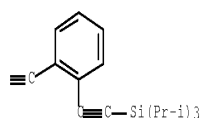
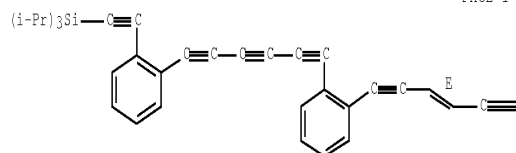
IT 214628-17-3P 214628-18-3P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(preparation of expanded planar dehydrobenzoannulenes with triacetylenic linkages)

RN 214628-17-8 CAPLUS

CN Silane, tris(1-methylethyl)[[2-[(3E)-6-[2-[4-[[tris(1-methylethyl)silyl]ethynyl]phenyl]-1,3-butadienyl]phenyl]-3-hexene-1,5-diynyl]phenyl]ethynyl]- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



RN 214628-18-9 CAPLUS

CN Silane, tris(1-methylethyl)[[2-[6-[2-[(3E)-6-[2-[[tris(1-methylethyl)silyl]ethynyl]phenyl]-3-hexene-1,5-diynyl]phenyl]-1,3,5-hexatriynyl]phenyl]ethynyl]- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

OS.CITING REF COUNT: 25 THERE ARE 25 CAPLUS RECORDS THAT CITE THIS RECORD (26 CITINGS)  
REFERENCE COUNT: 18 THERE ARE 18 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L7 ANSWER 27 OF 32 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1998:269262 CAPLUS [Full-text](#)

DOCUMENT NUMBER: 128:257221

ORIGINAL REFERENCE NO.: 128:50919a,50922a

TITLE: Steric Hindrance Facilitated Synthesis of Enynes and Their Intramolecular [4 + 2] Cycloaddition with Alkynes

AUTHOR(S): Gonzalez, Juan J.; Francesch, Andres; Cardenas, Diego J.; Echavarren, Antonio M.

CORPORATE SOURCE: Departamento de Química Organica, Universidad Autonoma de Madrid, Madrid, 28049, Spain

SOURCE: Journal of Organic Chemistry (1998), 63(9), 2854-2857  
CODEN: JOCEAH; ISSN: 0022-3263

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 128:257221

AB The palladium-catalyzed insertion of 1-alkynes into internal alkynes which are bent out of linearity by the interference with a peri or ortho substituent led to enynes regioselectively. The resulting enynes undergo a new type of intramol. thermal cycloaddn., which can be used for the annulation of an aryl ring onto naphthalene derivs. to afford fluranthenes. The cyclization of (E)-1-(1-buten-3-ynyl)-8-ethynyl naphthalene could also be performed in the presence of a Cu(I) catalyst at room temperature

IT 205124-39-6P

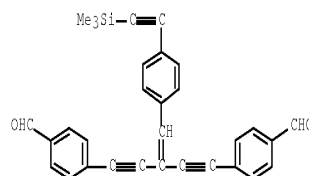
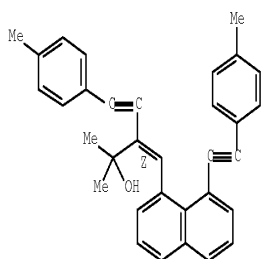
RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation of enynes and their intramol. [4+2]cycloaddn. with alkynes)

RN 205124-39-6 CAPLUS

CN 4-Pentyn-2-ol, 2-methyl-5-(4-methylphenyl)-3-[[8-[2-(4-methylphenyl)ethynyl]-1-naphthalenyl]methylene]-, (3Z)- (CA INDEX NAME)



Double bond geometry as shown.



OS.CITING REF COUNT: 22 THERE ARE 22 CAPLUS RECORDS THAT CITE THIS RECORD (22 CITINGS)  
REFERENCE COUNT: 47 THERE ARE 47 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L7 ANSWER 28 OF 32 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1998:247633 CAPLUS [Full-text](#)

DOCUMENT NUMBER: 128:295129

ORIGINAL REFERENCE NO.: 128:58501a,58504a

TITLE: Synthesis and characterization of well-defined fully conjugated hyperbranched oligomers of  $\beta,\beta$ -dibromo-4-ethynylstyrene

AUTHOR(S): Fomina, Lioudmila; Guadarrama, Patricia; Fomine, Serguei; Salcedo, Roberto; Ogawa, Takeshi

CORPORATE SOURCE: Instituto Investigaciones Materiales, Univ. Nacional Autonoma de Mexico, Mexico, 04510, Mex.

SOURCE: Polymer (1998), 39(12), 2629-2635

CODEN: POLMAG; ISSN: 0032-3861

PUBLISHER: Elsevier Science Ltd.

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Well-defined dendritic oligomers of poly( $\beta,\beta$ -dibromo-4-ethynylstyrene) of the first and second generation were synthesized by a stepwise synthesis, and characterized. NMR and theor. calcns. showed that free rotation around formal single bonds is hampered by conjugation. All of the oligomers were blue emitters with their emission maxima correlating with the number of repeating units. All dendrimers except  $\beta,\beta$ -bis[ $\beta',\beta'$ -di( $\beta'',\beta''$ -dibromostyryl-4"-ethynyl)styryl-4'-ethynyl]-4-ethynylstyrene showed two maxima in the excitation spectra.

IT 206181-71-7P 206181-72-8P 206181-73-9P

206181-74-0P 206181-75-1P 206181-76-2P

206181-77-3P 206181-78-4P

RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

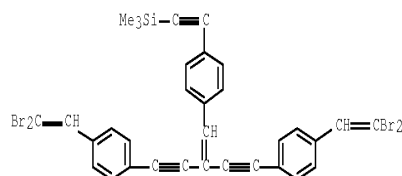
(preparation and characterization of conjugated hyperbranched  $\beta,\beta$ -dibromo-4-ethynylstyrene oligomers)

RN 206181-71-7 CAPLUS

CN Benzaldehyde, 4,4'-[3-[[4-[(trimethylsilyl)ethynyl]phenyl]methylene]-1,4-pentadiyne-1,5-diyl]bis- (9CI) (CA INDEX NAME)

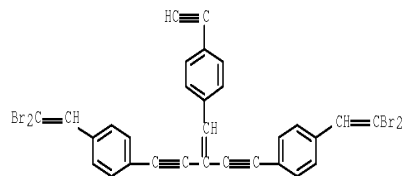
RN 206181-72-8 CAPLUS

CN Silane, [[4-[4-(2,2-dibromoethenyl)phenyl]-2-[[4-(2,2-dibromoethenyl)phenyl]ethynyl]-1-buten-3-ynyl]phenyl]ethynyl]trimethyl- (9CI) (CA INDEX NAME)



RN 206181-73-9 CAPLUS

CN Benzene, 1,1'-[3-[(4-ethynylphenyl)methylene]-1,4-pentadiyne-1,5-diyl]bis[4-(2,2-dibromoethenyl)- (9CI) (CA INDEX NAME)

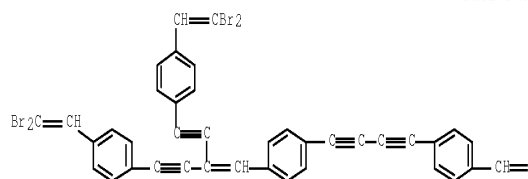


RN 206181-74-0 CAPLUS

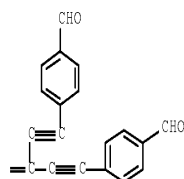
CN Benzene, 1,1'-[(1,3-butadiyne-1,4-diyl)bis[4-[4-(2,2-dibromoethenyl)phenyl]-2-[[4-(2,2-dibromoethenyl)phenyl]ethynyl]-1-buten-3-ynyl]- (9CI) (CA INDEX NAME)



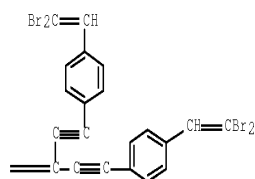
PAGE 1-A



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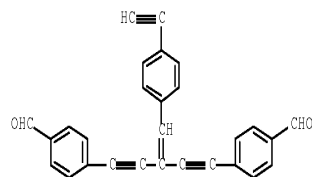


PAGE 1-B

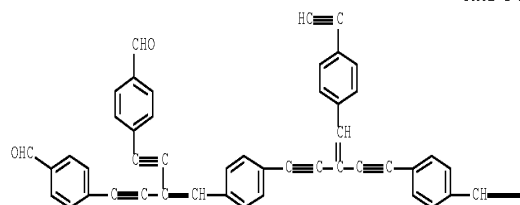


RN 206181-77-3 CAPLUS  
CN Benzaldehyde, 4,4'-[[3-[(4-ethynylphenyl)methylene]-1,4-pentadiyne-1,5-diyl]bis[4,1-phenylene[3-[(4-formylphenyl)ethynyl]-3-buten-1-yne-4,1-diyl]]bis- (9CI) (CA INDEX NAME)

RN 206181-75-1 CAPLUS  
CN Benzaldehyde, 4,4'-[[3-[(4-ethynylphenyl)methylene]-1,4-pentadiyne-1,5-diyl]bis- (CA INDEX NAME)



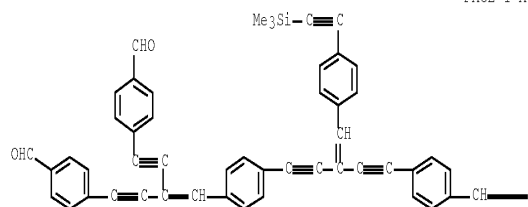
PAGE 1-A



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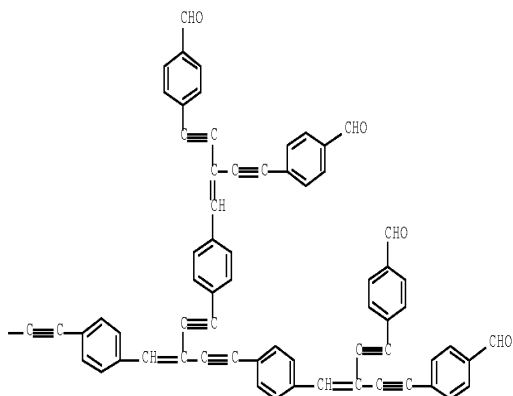
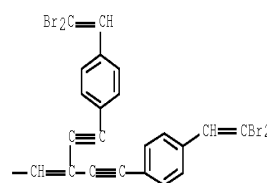
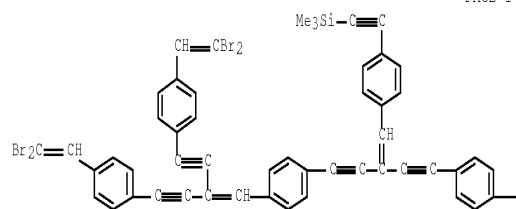
RN 206181-76-2 CAPLUS  
CN Benzaldehyde, 4,4'-[[3-[[4-[(trimethylsilyl)ethynyl]phenyl]methylene]-1,4-pentadiyne-1,5-diyl]bis[4,1-phenylene[3-[(4-formylphenyl)ethynyl]-3-buten-1-yne-4,1-diyl]]bis- (9CI) (CA INDEX NAME)

PAGE 1-A



RN 206181-78-4 CAPLUS  
CN Benzaldehyde, 4,4'-[[1,3-butadiyne-1,4-diyl]bis[4,1-phenylene[3-[[4-[(4-formylphenyl)-2-[(4-formylphenyl)ethynyl]-1-buten-3-ynyl]phenyl]ethynyl]-3-buten-1-yne-4,1-diyl]-4,1-phenylene[3-[(4-formylphenyl)ethynyl]-3-buten-1-yne-4,1-diyl]]bis- (9CI) (CA INDEX NAME)





OS.CITING REF COUNT: 11 THERE ARE 11 CAPLUS RECORDS THAT CITE THIS RECORD (11 CITINGS)

REFERENCE COUNT: 9 THERE ARE 9 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L7 ANSWER 29 OF 32 CAPLUS COPYRIGHT 2009 ACS ON STN

ACCESSION NUMBER: 1996:303100 CAPLUS [Full-text](#)

DOCUMENT NUMBER: 125:11582

ORIGINAL REFERENCE NO.: 125:2539a,2542a

TITLE: Synthesis and polymerization of  $\beta,\beta$ -dibromo-4-ethynylstyrene; preparation of a new polyconjugated, hyperbranched polymer

AUTHOR(S): Fomina, Lioudmila; Salcedo, Roberto

CORPORATE SOURCE: Inst. Investigaciones Materiales, Circuito Exterior, Ciudad Univ., Mexico City, 04510, Mex.

SOURCE: Polymer (1996), 37(9), 1723-1728

CODEN: POLMAG; ISSN: 0032-3861

PUBLISHER: Elsevier

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The monomer,  $\beta,\beta$ -dibromo-4-ethynylstyrene, was prepared and polymerized by the Heck reaction to give a partially soluble, conjugated hyperbranched polymer. The polymer structure was elucidated using standard spectroscopic techniques and with the aid of model compound synthesis. Theor. calcs. using the AM1 method were carried out and showed that conjugation in the polymer is partially disrupted by twisting of the benzene rings. Both the model compound and the polymer showed luminescence.

IT 177416-40-1P

RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)

IT 206181-79-5P

RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)  
(preparation and characterization of conjugated hyperbranched  $\beta,\beta$ -dibromo-4-ethynylstyrene oligomers)

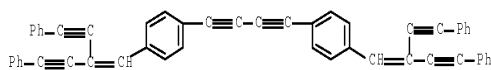
RN 206181-79-5 CAPLUS

CN Silane, [[4-[4-[4-[4-(2,2-dibromoethenyl)phenyl]-2-[[4-(2,2-dibromoethenyl)phenyl]ethynyl]-1-buten-3-ynyl]phenyl]-2-[[4-[4-(2,2-dibromoethenyl)phenyl]-2-[[4-(2,2-dibromoethenyl)phenyl]ethynyl]-1-buten-3-ynyl]phenyl]ethynyl]-1-buten-3-ynyl]phenyl]ethynyl]trimethyl- (9CI) (CA INDEX NAME)



(model compound for dibromoethynylstyrene polymer)

RN 177410-40-1 CAPLUS  
CN Benzene, 1,1'-(1,3-butadiyne-1,4-diyl)bis[4-[4-phenyl-2-(phenylethynyl)-1-buten-3-ynyl]- (9CI) (CA INDEX NAME)



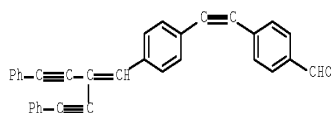
OS.CITING REF COUNT: 16 THERE ARE 16 CAPLUS RECORDS THAT CITE THIS RECORD (16 CITINGS)

L7 ANSWER 30 OF 32 CAPLUS COPYRIGHT 2009 ACS on STN  
ACCESSION NUMBER: 1995:946580 CAPLUS [Full-text](#)  
DOCUMENT NUMBER: 124:9540  
ORIGINAL REFERENCE NO.: 124:2031a,2034a  
TITLE: Novel polymers containing discrete conjugated units, produced by the Heck reaction  
AUTHOR(S): Fomine, Sergei; Fomina, Lioudmila; Florentino, Hector Quiroz; Mendez, Juan Manuel; Ogawa, Takeshi  
CORPORATE SOURCE: Instituto de Investigaciones en Materiales, Universidad Nacional Autonoma de Mexico, Coyoacan, 04510, Mex.  
SOURCE: Polymer Journal (Tokyo) (1995), 27(11), 1085-93  
CODEN: POLJB8; ISSN: 0032-3896  
PUBLISHER: Society of Polymer Science, Japan  
DOCUMENT TYPE: Journal  
LANGUAGE: English

AB Novel monomers and polymers containing arylenevinylideneethynylene groups were synthesized via the Heck reaction. The polymers were amorphous and soluble in common organic solvents. They have Tg .apprx.60°, 5% weight loss at 240-340° and undergo thermal crosslinking at 170-190° with loss of triple bonds. One of the polymers exhibits strong blue luminescence with emission maxima .apprx.380-390 and 470-480 nm with excitation at 320 nm. All polymers show 3rd order NLO susceptibility .apprx.10-10 esu.

IT 171296-95-3P  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(intermediate; in preparation of polyacetylene-polyesters)

RN 171296-95-0 CAPLUS  
CN Benzaldehyde, 4-[2-[4-[4-phenyl-2-(2-phenylethynyl)-1-buten-3-yn-1-yl]phenyl]ethynyl]- (CA INDEX NAME)

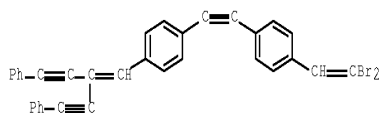


IT 171296-96-1P  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT

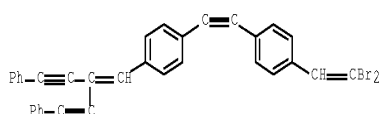
(Reactant or reagent)

(monomer; in preparation of polyacetylene-polyesters)

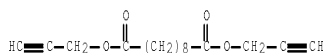
RN 171296-96-1 CAPLUS  
CN Benzene, 1-[2-[4-(2,2-dibromoethenyl)phenyl]ethynyl]-4-[4-phenyl-2-(2-phenylethynyl)-1-buten-3-yn-1-yl]- (CA INDEX NAME)



IT 171296-99-4P  
RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(preparation, characterization and properties of)  
RN 171296-99-4 CAPLUS  
CN Decanedioic acid, di-2-propynyl ester, polymer with 1-[[4-(2,2-dibromoethenyl)phenyl]ethynyl]-4-[4-phenyl-2-(phenylethynyl)-1-buten-3-ynyl]benzene (9CI) (CA INDEX NAME)  
CM 1  
CRN 171296-96-1  
CMF C34 H20 Br2

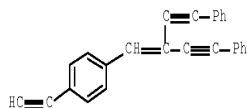


CM 2  
CRN 93164-22-8  
CMF C16 H22 O4



IT 171237-02-2,  $\beta,\beta$ -Bis(phenylethynyl)-4-ethynylstyrene  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(reactant; in preparation of polyacetylene-polyesters)  
RN 171297-02-2 CAPLUS  
CN Benzene, 1-ethynyl-4-[4-phenyl-2-(2-phenylethynyl)-1-buten-3-yn-1-yl]- (CA INDEX NAME)



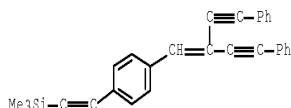


OS.CITING REF COUNT: 11 THERE ARE 11 CAPLUS RECORDS THAT CITE THIS RECORD (11 CITINGS)

L7 ANSWER 31 OF 32 CAPLUS COPYRIGHT 2009 ACS on STN  
 ACCESSION NUMBER: 1995:642218 CAPLUS [Full-text](#)  
 DOCUMENT NUMBER: 123:33763  
 ORIGINAL REFERENCE NO.: 123:6259a,6262a  
 TITLE: Synthesis and molten-state polymerization of some novel conjugated diacetylenes  
 AUTHOR(S): Fomina, Lioudmila; Allier, Hector; Fomine, Sergei; Salcedo, Roberto; Ogawa, Takeshi  
 CORPORATE SOURCE: Inst. Investigaciones Materiales, Ciudad Univ., Mexico, 04510, Mex.  
 SOURCE: Polymer Journal (Tokyo) (1995), 27(6), 591-600  
 CODEN: POLJB8; ISSN: 0032-3896  
 PUBLISHER: Society of Polymer Science, Japan  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English

AB A series of new, highly conjugated diacetylenes, 4-ethynylstilbene derivs., was synthesized and their polymerization was studied. None of them was found to undergo topochem. polymerization in the solid state but they readily polymerized in the molten state to give red transparent and amorphous polymers. All the polymers had an absorption maximum in the visible spectra around 500 nm, and FT-IR data showed the enyne structure of the polymer chain resulted from 1,4-addition

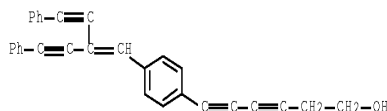
IT 164467-30-5P  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
 (in preparation of ethynylstilbene derivative monomers)  
 RN 164467-30-5 CAPLUS  
 CN Benzene, 1-[4-phenyl-2-(2-phenylethynyl)-1-buten-3-yn-1-yl]-4-[2-(trimethylsilyl)ethynyl]- (CA INDEX NAME)



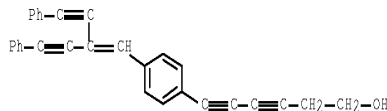
IT 164467-25-8P  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (preparation and characterization of polydiacetylenes from ethynylstilbene derivs. in molten state)  
 RN 164467-25-8 CAPLUS  
 CN 3,5-Hexadiyn-1-ol, 6-[4-[4-phenyl-2-(phenylethynyl)-1-buten-3-ynyl]phenyl]-

, homopolymer (9CI) (CA INDEX NAME)

CM 1  
 CRN 164467-20-3  
 CMF C30 H20 O



IT 164467-20-3P  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
 (preparation and polymerization of)  
 RN 164467-20-3 CAPLUS  
 CN 3,5-Hexadiyn-1-ol, 6-[4-[4-phenyl-2-(2-phenylethynyl)-1-buten-3-yn-1-yl]phenyl]- (CA INDEX NAME)



OS.CITING REF COUNT: 11 THERE ARE 11 CAPLUS RECORDS THAT CITE THIS RECORD (11 CITINGS)

L7 ANSWER 32 OF 32 CAPLUS COPYRIGHT 2009 ACS on STN  
 ACCESSION NUMBER: 1994:522234 CAPLUS [Full-text](#)  
 DOCUMENT NUMBER: 121:122234  
 ORIGINAL REFERENCE NO.: 121:21825h,21826a  
 TITLE: Difluoride derivative and liquid crystal composition containing the same  
 INVENTOR(S): Yokokoji, Osamu; Irisawa, Jun; Koh, Hidemasa  
 PATENT ASSIGNEE(S): Asahi Glass Co., Ltd., Japan  
 SOURCE: PCT Int. Appl., 43 pp.  
 CODEN: PIXXD2  
 DOCUMENT TYPE: Patent  
 LANGUAGE: Japanese  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9405613	A1	19940317	WO 1993-JP1235	19930901
W: US				
EP 628528	A1	19941214	EP 1993-919602	19930901
RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				



R: DE, FR, GB, IT

JP 06263661	A	19940920	JP 1993-219709	19930903
JP 3564711	B2	20040915		
US 5419851	A	19950530	US 1994-211625	19940420
JP 2004292454	A	20041021	JP 2004-115211	20040409
JP 3707493	B2	20051019		

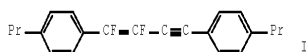
PRIORITY APPLN. INFO.:

		JP 1992-263027	A	19920904
		WO 1993-JP1235	W	19930901
		JP 1993-219709	A3	19930903

ASSIGNMENT HISTORY FOR US PATENT AVAILABLE IN LSUS DISPLAY FORMAT

OTHER SOURCE(S): MARPAT 121:122234

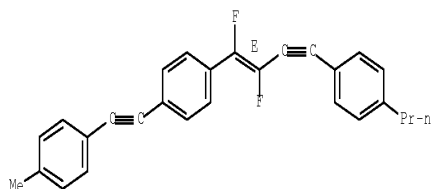
GI



AB Difluoride derivs. represented by the general formula:  
 $R1(A1Y1)mA2CF:CF: C.tplbond.CA3(Y2A4)nR2$  (A1 - A4 = trans-1,4-cyclohexylene, 1,4-cyclohexenylene, or 1,4-phenylene wherein  $\geq 1$  CH groups of each ring may be substituted by N or  $\geq 1$  CH<sub>2</sub> groups of the ring may be substituted by O or S; m, n = 0, 1; R1, R2 = C1-10 alkyl, halo, cyano wherein (1) O, CO<sub>2</sub>, or O<sub>2</sub>C may be inserted between the C-C bond of alkyl or that between alkyl and ring, (2) a part of the C-C bonds in alkyl is replaced by C:C or C.tplbond.C bond, or (3) one CH<sub>2</sub> group in alkyl is replaced by CO group; Y1, Y2 = CO<sub>2</sub>, O<sub>2</sub>C, C.tplbond.C, CH<sub>2</sub>CH<sub>2</sub>, CH:CH, OCH<sub>2</sub>, CH<sub>2</sub>O) are prepared These compds. have low viscosity, are light-stable, and hence can provide a liquid crystal composition having high response speed. Thus, 0.1 mol ClCF:CF<sub>2</sub> was blown into THF at -100° followed by adding dropwise 62.1 mL 1.61 M BuLi/hexane, stirring for 30 min, adding dropwise 0.1 mol Me<sub>3</sub>SiCl, stirring for 1 h, adding dropwise a solution of 4-propylphenyl lithium in THF (prepared from 4-propyliodobenzene and BuLi) at -100°, and stirring for 2 h at 0° to give 75% (Z)-4-PrC<sub>6</sub>H<sub>4</sub>CF:CFSiMe<sub>3</sub>. The latter compound (0.075 mol) was reacted with 0.15 mol KF in aqueous MeCN at 70° for 1 h to give 83% (E)-4-PrC<sub>6</sub>H<sub>4</sub>CF:CFH which (0.062 mol) was dissolved in THF, cooled to -78°, and treated dropwise with 38.5 mL 1.61 M BuLi/hexane followed by stirring for 30 min, adding 15.7 g iodine, and stirring at room temperature for 4 h to give 83% (E)-4-PrC<sub>6</sub>H<sub>4</sub>CF:CFI. The latter compound (0.051 mol) and 0.051 mol 4-propylphenylacetylene were dissolved in 100 mL Et<sub>3</sub>N followed by adding Pd(PPh<sub>3</sub>)<sub>2</sub>Cl<sub>2</sub> and CuI and the resulting mixture was allowed to react at room temperature for 6 h to give 70% diphenyldifluorobutenyne derivative (I). A STN-type liquid crystal display device was prepared from a liquid composition containing 20 weight% I and 80 weight% ZLI-1565 and irradiated with a UV carbon arc lamp for 200 h; new compds. were hardly formed whereas cis-4,4'-bis(n-propyl)difluorostilbene was formed in a liquid crystal composition containing ZLI-1565 and trans-4,4'-bis(n-propyl)difluorostilbene.

IT 156869-08-8P  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (preparation of, as liquid crystal with UV stability and low viscosity)  
 RN 156869-08-8 CAPLUS  
 CN Benzene, 1-[1,2-difluoro-4-(4-propylphenyl)-1-buten-3-ynyl]-4-[(4-methylphenyl)ethynyl]-, (E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

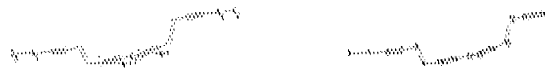


OS.CITING REF COUNT: 1 THERE ARE 1 CAPLUS RECORDS THAT CITE THIS RECORD (5 CITINGS)  
 REFERENCE COUNT: 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

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 chain bonds :  
 4-5 5-6 6-7 7-8 8-9 9-10 10-11 11-12 12-13 13-14 14-15 15-16 16-17 17-18  
 18-19 19-20  
 exact/norm bonds :  
 4-5 5-6 11-12 12-13 18-19 19-20  
 exact bonds :  
 6-7 7-8 8-9 9-10 10-11 13-14 14-15 15-16 16-17 17-18

G1:Cb,Cy,Hy

G2:C,H,O,N,Cl,Br,F,I

G3:C,H,Si,Cb,Cy,Hy

Match level :  
 4:CLASS 5:CLASS 6:CLASS 7:CLASS 8:CLASS 9:CLASS 10:CLASS 11:CLASS 12:CLASS  
 13:CLASS 14:CLASS 15:CLASS 16:CLASS 17:CLASS 18:CLASS 19:CLASS 20:CLASS



L8 STRUCTURE UPLOADED

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FULL SCREEN SEARCH COMPLETED - 11728 TO ITERATE

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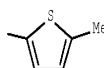
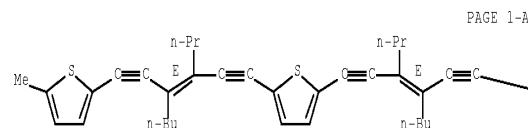
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L10 ANSWER 1 OF 22 CAPLUS COPYRIGHT 2009 ACS on STN  
ACCESSION NUMBER: 2009:1099083 CAPLUS Full-text  
DOCUMENT NUMBER: 151:508432  
TITLE: Hybrid Conjugated Organic Oligomers Consisting of  
Oligodiacetylene and Thiophene Units: Synthesis and  
Optical Properties  
AUTHOR(S): Pilzak, Gregor S.; van Grujthuijsen, Kitty; van  
Doorn, Reindert H.; van Lagen, Barend; Sudhoelter,  
Ernst J. R.; Zuilhof, Han  
CORPORATE SOURCE: Laboratory of Organic Chemistry, Wageningen  
University, Dreijenplein 8, Wageningen, 6703 HB, Neth.  
SOURCE: Chemistry--A European Journal (2009), 15(36),  
9085-9096, S9085/1-S9085/19  
CODEN: CEUJED; ISSN: 0947-6539  
PUBLISHER: Wiley-VCH Verlag GmbH & Co. KGaA  
DOCUMENT TYPE: Journal  
LANGUAGE: English  
OTHER SOURCE(S): CASREACT 151:508432  
AB Novel and highly soluble hybrid conjugated organic oligomers consisting of  
oligodiacetylene and thiophene units have been synthesized in high purity  
through iterative and divergent approaches based on a sequence of Sonogashira  
reactions. The series of thiophene-containing oligodiacetylenes and  
homocoupled oligodiacetylenes show, both in solution and in the solid state, a  
strong optical absorption, which is progressively red shifted with increasing  
chain length. The linear correlation of the absorption maximum with the  
inverse of conjugation length (CL = number of double and triple bonds) shows  
that the effective conjugation length of this system is extended up to at  
least CL = 20. Furthermore, absorption measurements of dropcast thin films  
display not only a bathochromic shift of the absorption maxima but also a  
higher wavelength absorption, which is attributed to increased  $\pi$ - $\pi$   
interactions. The wavelength of the maximum fluorescence emission also  
increases with CL, and emission is maximal for oligomers with CL = 7-12  
(fluorescence quantum yield  $\Phi_F$  = .apprx.0.2). Both longer and shorter  
oligomers display marginal emission. The calculated Stokes shifts of these  
planar materials are relatively large (0.4 eV) for all oligomers, and likely  
due to excitation to the S2 state, thus suggesting that the presence of enyne  
moieties dominates the ordering of the lowest excited states. The  
fluorescence lifetimes ( $\tau_F$ ) are short ( $\tau_{Fmax}$  =  $\approx$ 1 ns) and closely follow the

tendency obtained for the fluorescence quantum yield. The anisotropy  
lifetimes show a near-linear increase with CL in line with highly rigid  
oligomers.

IT 1192820-79-3P  
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)  
(synthesis via iterative Sonogashira coupling and optical properties of  
hybrid conjugated organic oligomers consisting of oligodiacetylene and  
thiophene units)  
RN 1192820-79-3 CAPLUS  
CN INDEX NAME NOT YET ASSIGNED

Double bond geometry as shown.



REFERENCE COUNT: 56 THERE ARE 56 CITED REFERENCES AVAILABLE FOR THIS  
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L10 ANSWER 2 OF 22 CAPLUS COPYRIGHT 2009 ACS on STN  
ACCESSION NUMBER: 2009:76616 CAPLUS Full-text  
DOCUMENT NUMBER: 150:167710  
TITLE: Push-pull hyperbranched molecules. A theoretical study  
AUTHOR(S): Ramos, Estrella; Guadarrama, Patricia; Teran, Gerardo;  
Fomine, Serguei  
CORPORATE SOURCE: Instituto de Investigaciones en Materiales,  
Universidad Nacional Autonoma de Mexico, Mexico,  
04510, Mex.  
SOURCE: Journal of Physical Organic Chemistry (2009), 22(1),  
9-16  
CODEN: JPOCEE; ISSN: 0894-3230  
PUBLISHER: John Wiley & Sons Ltd.  
DOCUMENT TYPE: Journal  
LANGUAGE: English  
AB The electronic properties of the ground state, unrelaxed and relaxed first  
excited states of push-pull hyperbranched mols. bearing amino and nitro  
terminal groups have been studied at BB1K/cc-pvdz//HF/6-31g(d), TD-BB1K/cc-  
pvdz//HF/6-31g(d) and TD-BB1K/cc-pvdz//CIS/6-31g(d) levels of theory, resp.  
It was demonstrated that dendritic architecture of push-pull mols. favors the  
charge transfer in the excited state compared to linear mols. The possibility  
of adopting a plane conformation is an important condition for the charge  
transfer in an excited state. According to the calcs. 1:1 ratio of donor and  
acceptor groups is another important precondition for the manifestation of



strong charge separation in the excited state. In case of excess of nitro groups over the amino, some of the excitations participating in the  $S_0 \rightarrow S_1$  transition favor the charge transfer in the excited state in the opposite directions, thus decreasing the charge separation

PAGE 1-B

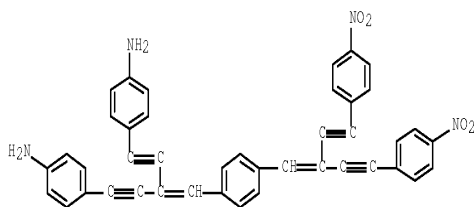
IT 1107616-70-5 1107616-72-7

RL: PRP (Properties)

(electronic properties of ground state, unrelaxed and relaxed first excited states of push-pull hyperbranched mols. bearing amino and nitro terminal groups)

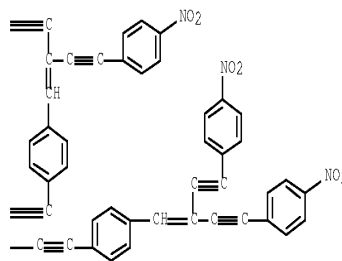
RN 1107616-70-5 CAPLUS

CN Benzenamine, 4,4'-[3-[[4-[4-(4-nitrophenyl)-2-[2-(4-nitrophenyl)ethynyl]-1-buten-3-yn-1-yl]phenyl]methylene]-1,4-pentadiyne-1,5-diyl]bis- (CA INDEX NAME)



RN 1107616-72-7 CAPLUS

CN Benzenamine, 4,4'-[3-[[4-[5-[4-[4-(4-aminophenyl)-2-[2-(4-aminophenyl)ethynyl]-1-buten-3-yn-1-yl]phenyl]-3-[[4-[4-[4-(4-nitrophenyl)-2-[2-(4-nitrophenyl)ethynyl]-1-buten-3-yn-1-yl]phenyl]-2-[2-[4-[4-(4-nitrophenyl)-2-[2-(4-nitrophenyl)ethynyl]-1-buten-3-yn-1-yl]phenyl]ethynyl]-1-buten-3-yn-1-yl]phenyl]methylene]-1,4-pentadiyn-1-yl]phenyl]methylene]-1,4-pentadiyne-1,5-diyl]bis- (CA INDEX NAME)



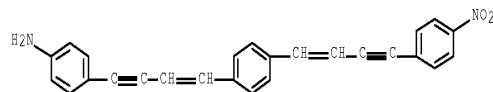
IT 1107616-75-0 1107616-76-1

RL: PRP (Properties)

(linear analog; electronic properties of ground state, unrelaxed and relaxed first excited states of push-pull hyperbranched mols. bearing amino and nitro terminal groups)

RN 1107616-75-0 CAPLUS

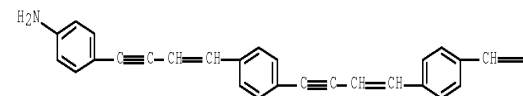
CN Benzenamine, 4-[4-[4-[4-(4-nitrophenyl)-1-buten-3-yn-1-yl]phenyl]-3-buten-1-yn-1-yl]- (CA INDEX NAME)



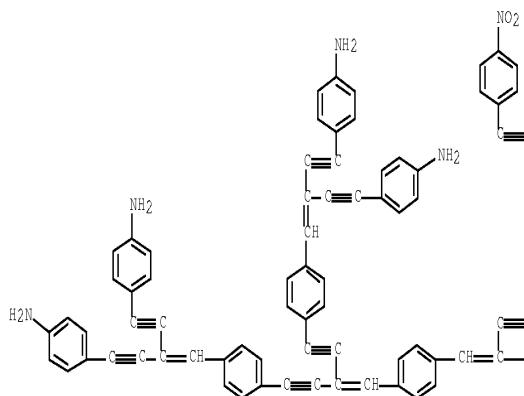
RN 1107616-76-1 CAPLUS

CN Benzenamine, 4-[4-[4-[4-[4-[4-[4-(4-nitrophenyl)-1-buten-3-yn-1-yl]phenyl]-1-buten-3-yn-1-yl]phenyl]-3-buten-1-yn-1-yl]phenyl]-3-buten-1-yn-1-yl]- (CA INDEX NAME)

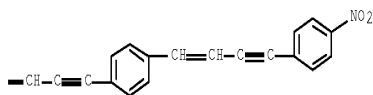
PAGE 1-A



PAGE 1-A







REFERENCE COUNT: 21 THERE ARE 21 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L10 ANSWER 3 OF 22 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 2008:244421 CAPLUS [Full-text](#)

DOCUMENT NUMBER: 148:403337

TITLE: Triphenylphosphine Incorporation Reactions of Diynyl Complexes Containing a  $\text{TpRu}(\text{NO})$  Fragment and Isomerization to Ruthenacyclobuta[b]naphthalene  
 AUTHOR(S): Arikawa, Yasuhiro; Asayama, Taiki; Tanaka, Chie; Tashita, Shin-ya; Tsuji, Misako; Ikeda, Kenta; Umakoshi, Keisuke; Onishi, Masayoshi

CORPORATE SOURCE: Department of Applied Chemistry, Faculty of Engineering, Nagasaki University, Nagasaki, 852-8521, Japan

SOURCE: Organometallics (2008), 27(6), 1227-1233  
 CODEN: ORGND7; ISSN: 0276-7333

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 148:403337

AB Nitrosylruthenium arylbutadiynyl complexes having a Tp ligand (Tp = BH(pyrazol-1-yl)<sub>3</sub>) were prepared, and their reactivities toward PPh<sub>3</sub> incorporation in the presence of HBF<sub>4</sub>·Et<sub>2</sub>O were described. The PPh<sub>3</sub> incorporation of mono(arylbutadiynyl) complex  $\text{TpRuCl}(\text{C.tplbond.C-C.tplbond.C-C6H4Me})(\text{NO})$  (1) resulted in the  $\beta$ -phosphonioalkenyl complex (E)-[ $\text{TpRuCl}(\text{CH:C}(\text{PPh}_3)\text{-C.tplbond.C-C6H4Me})(\text{NO})\text{]BF}_4$  (2·BF<sub>4</sub>), whereas when bis(arylbutadiynyl)  $\text{TpRu}(\text{C.tplbond.C-C.tplbond.C-C6H4Me})_2(\text{NO})$  (3) was treated, mono- and bis( $\beta$ -phosphonioalkenyl) complexes (E)-[ $\text{TpRu}(\text{C.tplbond.C-C.tplbond.C-C6H4Me})(\text{CH:C}(\text{PPh}_3)\text{-C.tplbond.C-C6H4Me})(\text{NO})\text{]BF}_4$  (4·BF<sub>4</sub>) and (E,E)-[ $\text{TpRu}(\text{CH:C}(\text{PPh}_3)\text{-C.tplbond.C-C6H4Me})_2(\text{NO})\text{]BF}_4$  (5·BF<sub>4</sub>) were obtained depending on the reaction conditions. On the other hand, an unsym. mixed (arylbutadiynyl)(3-hydroxyalkynyl) complex,  $\text{TpRu}(\text{C.tplbond.C-C.tplbond.C-C6H4Me})(\text{C.tplbond.CCPh}_2(\text{OH}))(\text{NO})$  (6), was allowed to react with PPh<sub>3</sub> in the presence of the protic acid to give the  $\alpha$ -phosphonioallenyl [ $\text{TpRu}(\text{C.tplbond.C-C.tplbond.C-C6H4Me})(\text{C}(\text{PPh}_3)\text{:C:CPH}_2)(\text{NO})\text{]BF}_4$  (7·BF<sub>4</sub>). Interestingly, thermal isomerization of 7·BF<sub>4</sub> to a ruthena-2-PPh<sub>3</sub>-cyclobuta[b]naphthalene [ $\text{TpRu}(\text{CH}(\text{PPh}_3)[3\text{-Ph-8-(MeC6H4-C.tplbond.C)-ClOH4}])\text{]BF}_4$  (8·BF<sub>4</sub>) was observed

IT 1515477-39-1F

RL: SPN (Synthetic preparation); PREP (Preparation)  
 (triphenylphosphine incorporation reactions of diynyl complexes containing pyrazolylboratoruthenium nitrosyl fragment and isomerization to ruthenacyclobutanaphthalene)

RN 1015477-30-1 CAPLUS

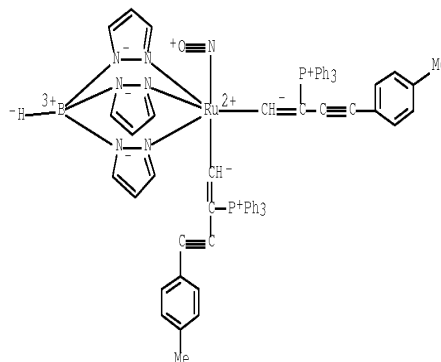
CN Ruthenium(2+), [hydrotris(1H-pyrazolato- $\kappa\text{N1}$ )borato(1-)- $\kappa\text{N2}, \kappa\text{N2}', \kappa\text{N2}''$ ]bis[(1E)-4-(4-methylphenyl)-2-(triphenylphosphonio)-1-buten-3-yn-1-yl]nitrosyl-, (OC-6-23)-, tetrafluoroborate(1-)(1:2) (CA INDEX NAME)

CM 1

CRN 1015477-29-8

CMF C67 H56 B N7 O P2 Ru

CCI CCS



CM 2

CRN 14874-70-5

CMF B F4

CCI CCS



OS.CITING REF COUNT: 5 THERE ARE 5 CAPLUS RECORDS THAT CITE THIS RECORD (5 CITINGS)

REFERENCE COUNT: 41 THERE ARE 41 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L10 ANSWER 4 OF 22 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 2008:112838 CAPLUS [Full-text](#)

DOCUMENT NUMBER: 148:331583

TITLE: 3-iodo-3-trimethylsilylpropenal as a useful unit for pinacol coupling and subsequent functional group transformations

AUTHOR(S): Shimizu, Makoto; Okimura, Hisashi; Manabe, Nobuyuki; Hachiya, Iwao

CORPORATE SOURCE: Department of Chemistry for Materials, Graduate School of Engineering, Mie University, Tsu, 514-8507, Japan

SOURCE: Chemistry Letters (2008), 37(1), 28-29

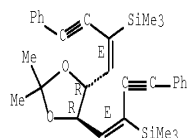
CODEN: CMLTAG; ISSN: 0366-7022

PUBLISHER: Chemical Society of Japan



DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 OTHER SOURCE(S): CASREACT 148:331583  
 AB Stereoselective titanium tetraiodide-promoted pinacol coupling reactions of (Z)-3-halo-3-(substituted-silyl)prop-2-en-1-als are used for the preparation of trans-4,5-bis[(Z)-2-halo-2-(substituted-silyl)vinyl]-2,2-dimethyl-1,3-dioxolanes. These dioxolanes are then used for subsequent C-C bond-forming reactions.  
 IT 1011296-76-6P  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (3-halo-3-(substituted-silyl)prop-2-en-1-als as reactants for stereoselective pinacol coupling to form bis-substituted dioxolanes)  
 RN 1011296-76-6 CAPLUS  
 CN 1,3-Dioxolane, 2,2-dimethyl-4,5-bis[(1E)-4-phenyl-2-(trimethylsilyl)-1-buten-3-yn-1-yl]-, (4R,5R)-rel- (CA INDEX NAME)

Relative stereochemistry.  
 Double bond geometry as shown.

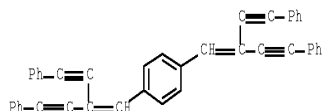


OS.CITING REF COUNT: 2 THERE ARE 2 CAPLUS RECORDS THAT CITE THIS RECORD (2 CITINGS)  
 REFERENCE COUNT: 21 THERE ARE 21 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

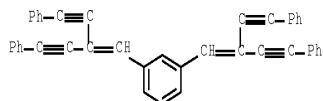
L10 ANSWER 5 OF 22 CAPLUS COPYRIGHT 2009 ACS on STN  
 ACCESSION NUMBER: 2007:939644 CAPLUS [Full-text](#)  
 DOCUMENT NUMBER: 147:385553  
 TITLE: EDA Study of  $\pi$ -Conjugation in Tunable Bis(gem-diethynylethene) Fluorophores  
 AUTHOR(S): Fernandez, Israel; Frenking, Gernot  
 CORPORATE SOURCE: Fachbereich Chemie, Philipps-Universitaet Marburg, Marburg, D-35043, Germany  
 SOURCE: Journal of Organic Chemistry (2007), 72(19), 7367-7372  
 CODEN: JOCEAH; ISSN: 0022-3263  
 PUBLISHER: American Chemical Society  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English

AB The strength of  $\pi$ -conjugation in a family of bis(gem-diethynylethene) fluorophores is estimated within the d. functional theory framework using the energy decomposition anal. (EDA) method. The observed very good linear correlations between the calculated  $\pi$ -conjugation and the exptl. values for the UV absorption and fluorescence emission for this series of compds. suggest that the values given by the EDA are useful for the interpretation and prediction of photochem. properties of the mols. The calculated data predict that adequate modifications in the core moiety of the mol. such as  $\pi$ -donor substituents in the aromatic ring or in the periphery of the bis-enediyne unit like  $\pi$ -acceptor groups placed in the para position of the aryl substituent increase the total  $\pi$ -conjugation in the systems and thus provoke significant

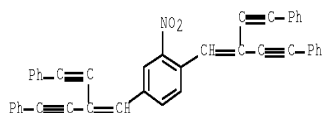
changes in both the absorption and emission spectra leading to large Stokes shifts. The effect of such substituents is quant. predicted by the EDA data.  
 IT 360549-89-9 610283-06-2 610283-08-4  
 610283-03-5 610283-10-8 610283-12-9  
 350584-33-6  
 RL: PRP (Properties)  
 (experiment and calcn.; EDA study of  $\pi$ -conjugation in tunable bis(gem-diethynylethene) fluorophores)  
 RN 360549-89-9 CAPLUS  
 CN Benzene, 1,4-bis[4-phenyl-2-(2-phenylethynyl)-1-buten-3-yn-1-yl]- (CA INDEX NAME)



RN 610283-06-2 CAPLUS  
 CN Benzene, 1,3-bis[4-phenyl-2-(2-phenylethynyl)-1-buten-3-yn-1-yl]- (CA INDEX NAME)

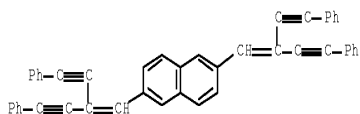


RN 610283-08-4 CAPLUS  
 CN Benzene, 2-nitro-1,4-bis[4-phenyl-2-(2-phenylethynyl)-1-buten-3-yn-1-yl]- (CA INDEX NAME)

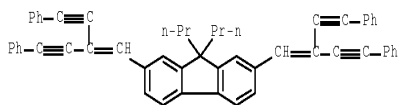


RN 610283-09-5 CAPLUS  
 CN Naphthalene, 2,6-bis[4-phenyl-2-(2-phenylethynyl)-1-buten-3-yn-1-yl]- (CA INDEX NAME)

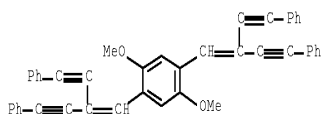




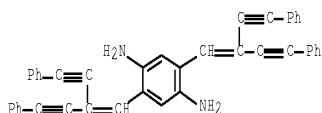
RN 610283-10-8 CAPLUS  
CN 9H-Fluorene, 2,7-bis[4-phenyl-2-(2-phenylethynyl)-1-buten-3-yn-1-yl]-9,9-dipropyl- (CA INDEX NAME)



RN 610283-12-0 CAPLUS  
CN Benzene, 1,4-dimethoxy-2,5-bis[4-phenyl-2-(2-phenylethynyl)-1-buten-3-yn-1-yl]- (CA INDEX NAME)



RN 950584-34-6 CAPLUS  
CN 1,4-Benzenediamine, 2,5-bis[4-phenyl-2-(2-phenylethynyl)-1-buten-3-yn-1-yl]- (CA INDEX NAME)



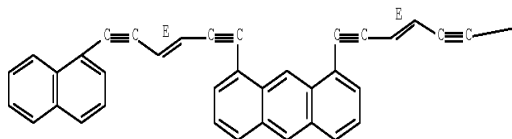
OS.CITING REF COUNT: 2 THERE ARE 2 CAPLUS RECORDS THAT CITE THIS RECORD (2 CITINGS)  
REFERENCE COUNT: 28 THERE ARE 28 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L10 ANSWER 6 OF 22 CAPLUS COPYRIGHT 2009 ACS on STN  
ACCESSION NUMBER: 2007:46877 CAPLUS [Full-text](#)  
DOCUMENT NUMBER: 148:284829  
TITLE: Synthesis of smallest unit model of graphite

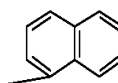
intercalation compound and its possibility  
AUTHOR(S): Ogoshi, Sensuke  
CORPORATE SOURCE: Department of Applied Chemistry, Faculty of Engineering, Osaka University, Japan  
SOURCE: Asahi Garasu Zaidan Josei Kenkyu Seika Hokoku (2006) 01.03.07/1-01.03.07/8  
CODEN: AGSHEN; ISSN: 0919-9179  
PUBLISHER: Asahi Garasu Zaidan  
DOCUMENT TYPE: Journal; (computer optical disk)  
LANGUAGE: Japanese  
OTHER SOURCE(S): CASREACT 148:284829  
AB Graphite is perhaps the simplest layered structure. Many substances can be intercalated between layers of graphite. Upon intercalation, the graphite layers moved apart somewhat due to the intercalated atom. However, the layers still keep parallel each other which would be the key for the formation of intercalation compds. Thus, compds. having two aromatic rings, which can change the distance between the rings and keep parallel to each other, were designed and synthesized. The target compound was 1,8-bis[6-(1-naphthalenyl)-3-hexene-1,5-diynyl]anthracene.  
IT 1007602-95-02  
RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation of bis[(naphthalenyl)hexenediynyl]anthracene (smallest unit model for graphite intercalation compound))  
RN 1007602-95-0 CAPLUS  
CN Anthracene, 1,8-bis[(3E)-6-(1-naphthalenyl)-3-hexene-1,5-diyn-1-yl]- (CA INDEX NAME)

Double bond geometry as shown.

PAGE 1-A



PAGE 1-B



L10 ANSWER 7 OF 22 CAPLUS COPYRIGHT 2009 ACS on STN  
ACCESSION NUMBER: 2005:1004691 CAPLUS [Full-text](#)  
DOCUMENT NUMBER: 143:306181  
TITLE: Process for preparation of  $\pi$ -conjugated aromatic ring-containing acetylene derivatives as organic electroluminescent devices



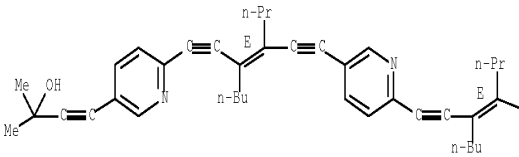
INVENTOR(S): Sato, Fumie; Takayama, Yuuki  
PATENT ASSIGNEE(S): Nissan Chemical Industries, Ltd., Japan  
SOURCE: PCT Int. Appl., 82 pp.  
CODEN: PIXXD2  
DOCUMENT TYPE: Patent  
LANGUAGE: Japanese  
FAMILY ACC. NUM. COUNT: 1  
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005085176	A1	20050915	WO 2005-JP3950	20050308
W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW			
RW:	BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG			

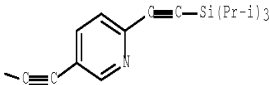
US 20070176164 A1 20070802 US 2007-591950 20070307  
PRIORITY APPLN. INFO.: JP 2004-65446 A 20040309  
WO 2005-JP3950 W 20050308

ASSIGNMENT HISTORY FOR US PATENT AVAILABLE IN LSUS DISPLAY FORMAT

OTHER SOURCE(S): MARPAT 143:306181  
GI



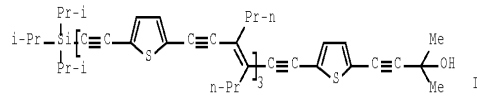
PAGE 1-A



PAGE 1-B

RN 740810-68-8 CAPLUS  
CN 3-Butyn-2-ol, 2-methyl-4-[5-[(3E)-3-propyl-4-[[5-[(3E)-3-propyl-4-[[5-[[tris(1-methylethyl)silyl]ethynyl]-2-thienyl]ethynyl]-3-hepten-1-yn-1-yl]-2-thienyl]ethynyl]-3-hepten-1-yn-1-yl]-2-thienyl]- (CA INDEX NAME)

Double bond geometry as shown.



AB This invention pertains to a method for producing  $\pi$ -conjugated aromatic ring-containing acetylene derivs. via coupling reaction in the presence of palladium and Cu(I) catalysts. For example, the compound I was prepared in a multi-step synthesis in good yield. The title compds. are useful as electroluminescent devices.

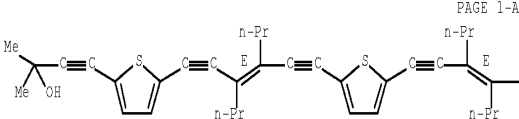
IT 740810-65-5P 740810-65-5P 864683-97-6P  
864683-97-6P

RL: IMF (Industrial manufacture); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(intermediate; preparation of  $\pi$ -conjugated aromatic ring-containing acetylene derivs. as organic electroluminescent devices)

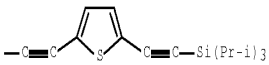
RN 740810-65-5 CAPLUS

CN 3-Butyn-2-ol, 4-[6-[(3E)-3-butyl-4-[2-[6-[(3E)-3-butyl-4-[2-[6-[2-[tris(1-methylethyl)silyl]ethynyl]-3-pyridinyl]ethynyl]-3-hepten-1-yn-1-yl]-3-pyridinyl]ethynyl]-3-hepten-1-yn-1-yl]-2-methyl- (CA INDEX NAME)

Double bond geometry as shown.



PAGE 1-A

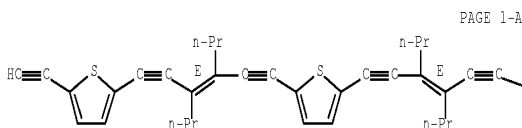


PAGE 1-B

RN 864683-97-6 CAPLUS  
CN 3-Butyn-2-ol, 4-[5-[(3E)-4-[2-[5-[(3E)-4-[2-(5-ethynyl-2-thienyl)ethynyl]-3-propyl-3-hepten-1-yn-1-yl]-2-thienyl]ethynyl]-3-propyl-3-hepten-1-yn-1-yl]-2-thienyl]-2-methyl- (CA INDEX NAME)

Double bond geometry as shown.

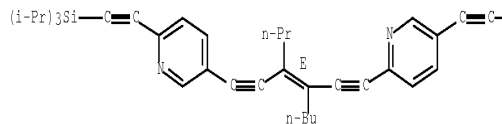




RN 740810-66-6 CAPLUS  
 CN 3-Butyn-2-ol, 4-[6-[(3E)-3-butyl-4-[2-[6-[(3E)-3-butyl-4-[2-[6-[(3E)-3-butyl-4-[2-[6-[tris(1-methylethyl)silyl]ethynyl]-3-pyridinyl]ethynyl]-3-hepten-1-yn-1-yl]-3-pyridinyl]ethynyl]-3-hepten-1-yn-1-yl]-3-pyridinyl]ethynyl]-3-hepten-1-yn-1-yl]-3-pyridinyl]-2-methyl- (CA INDEX NAME)

Double bond geometry as shown.

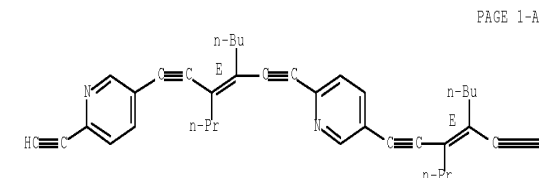
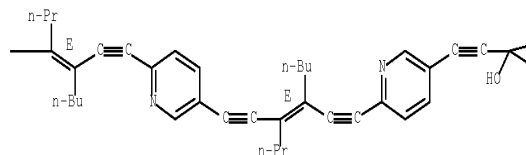
PAGE 1-A



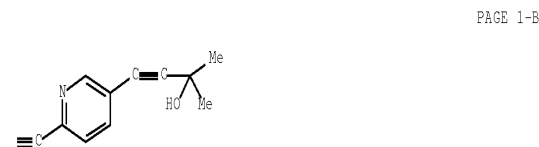
RN 864684-02-6 CAPLUS  
 CN 3-Butyn-2-ol, 4-[6-[(3E)-3-butyl-4-[2-[6-[(3E)-3-butyl-4-[2-(6-ethynyl-3-pyridinyl)ethynyl]-3-hepten-1-yn-1-yl]-3-pyridinyl]ethynyl]-3-hepten-1-yn-1-yl]-3-pyridinyl]-2-methyl- (CA INDEX NAME)

Double bond geometry as shown.

PAGE 1-B



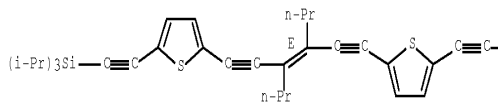
PAGE 1-C



RN 740810-69-9 CAPLUS  
 CN 3-Butyn-2-ol, 4-[5-[(3E)-4-[2-[5-[(3E)-5-ethyl-4-[2-[5-[(3E)-5-ethyl-3-propyl-4-[2-[5-[2-[tris(1-methylethyl)silyl]ethynyl]-2-thienyl]ethynyl]-3-penten-1-yn-1-yl]-2-thienyl]ethynyl]-3-propyl-3-penten-1-yn-1-yl]-2-thienyl]ethynyl]-3-propyl-3-hepten-1-yn-1-yl]-2-thienyl]-2-methyl- (CA INDEX NAME)

Double bond geometry as shown.

PAGE 1-A



IT 740810-66-6P 740810-69-9P 864684-02-6P  
 864684-03-3P 864684-21-3P 864684-22-3P  
 864684-23-1P 864684-26-4P 864684-27-5P  
 864684-28-6P 864684-29-7P 864684-30-0P  
 RL: DEV (Device component use); IMF (Industrial manufacture); SPN  
 (Synthetic preparation); TEM (Technical or engineered material use); PREP  
 (Preparation); USES (Uses)  
 (preparation of  $\pi$ -conjugated aromatic ring-containing acetylene derivs. as  
 organic electroluminescent devices)



\*C(=C(C)C)C#CC1=CC=C(C=C1)C#CC2=CC=C(C=C2)C#CC3=CC=C(C=C3)C#CC4(C)C(O)C5=CC=CC=C5C4

Me

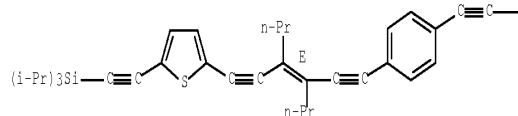
CN 2,1,3-Benzothiadiazole, 4-[(3E)-3,4-dipropyl-6-[5-[2-[tris(1-methylethyl)silyl]ethynyl]-2-thienyl]-3-hexene-1,5-diyn-1-yl]-7-[(3E)-3-propyl-4-[2-[5-[2-[tris(1-methylethyl)silyl]ethynyl]-2-thienyl]ethynyl]-3-hepten-1-yn-1-yl]- (CA INDEX NAME)

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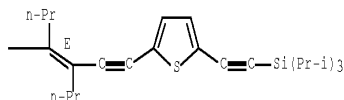
CN Thieno[3,4-b]pyrazine, 5-[(3E)-3,4-dipropyl-6-(2-thienyl)-3-hexene-1,5-diyn-1-yl]-2,3-diphenyl-7-[(3E)-3-propyl-4-[2-(2-thienyl)ethynyl]-3-hepten-1-yn-1-yl]- (CA INDEX NAME)

CN Thiophene, 2-[(3E)-3,4-dipropyl-6-[4-[(3E)-3-propyl-4-[2-[5-[2-[tris(1-methylethyl)silyl]ethynyl]-2-thienyl]ethynyl]-3-hepten-1-yn-1-yl]phenyl]-3-hexene-1,5-diyn-1-yl]-5-[2-[tris(1-methylethyl)silyl]ethynyl]- (CA INDEX NAME)

PAGE 1-A

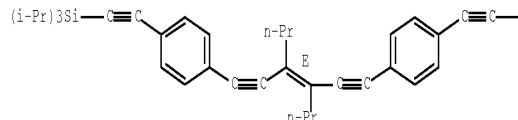


PAGE 1-B

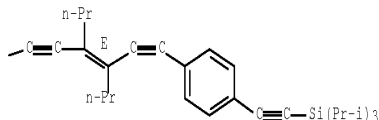
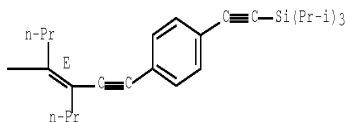


CN Benzene, 1-[(3E)-3,4-dipropyl-6-[4-[2-[tris(1-methylethyl)silyl]ethynyl]phenyl]-3-hexene-1,5-diyn-1-yl]-4-[(3E)-3-propyl-4-[2-[4-[2-[tris(1-methylethyl)silyl]ethynyl]phenyl]ethynyl]-3-hepten-1-yn-1-yl]- (CA INDEX NAME)

PAGE 1-A



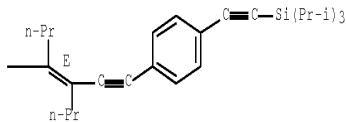
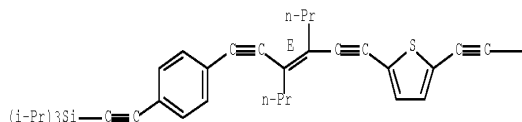




RN 864684-23-1 CAPLUS

CN Thiophene, 2-[(3E)-3,4-dipropyl-6-[4-[2-[tris(1-methylethyl)silyl]ethynyl]phenyl]-3-hexene-1,5-diyn-1-yl]-5-[(3E)-3-propyl-4-[2-[4-[2-[tris(1-methylethyl)silyl]ethynyl]phenyl]ethynyl]-3-hepten-1-yn-1-yl]- (CA INDEX NAME)

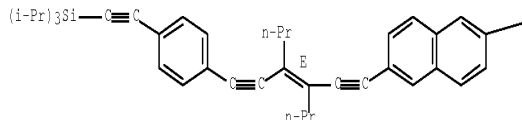
Double bond geometry as shown.



RN 864684-26-4 CAPLUS

CN Naphthalene, 2-[(3E)-3,4-dipropyl-6-[4-[2-[tris(1-methylethyl)silyl]ethynyl]phenyl]-3-hexene-1,5-diyn-1-yl]-6-[(3E)-3-propyl-4-[2-[4-[2-[tris(1-methylethyl)silyl]ethynyl]phenyl]ethynyl]-3-hepten-1-yn-1-yl]- (CA INDEX NAME)

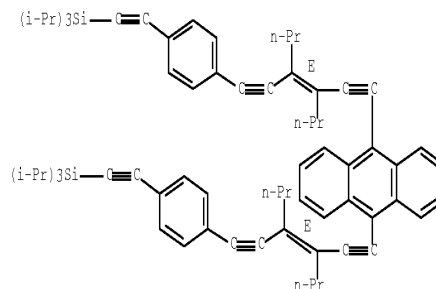
Double bond geometry as shown.



RN 864684-27-5 CAPLUS

CN Anthracene, 9-[(3E)-3,4-dipropyl-6-[4-[2-[tris(1-methylethyl)silyl]ethynyl]phenyl]-3-hexene-1,5-diyn-1-yl]-10-[(3E)-3-propyl-4-[2-[4-[2-[tris(1-methylethyl)silyl]ethynyl]phenyl]ethynyl]-3-hepten-1-yn-1-yl]- (CA INDEX NAME)

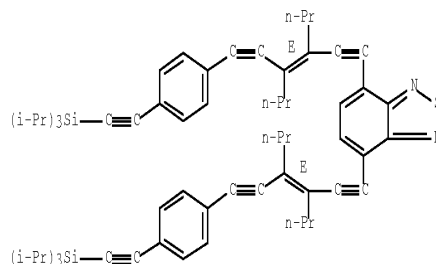
Double bond geometry as shown.



RN 864684-28-6 CAPLUS

CN 2,1,3-Benzothiadiazole, 4-[(3E)-3,4-dipropyl-6-[4-[2-[tris(1-methylethyl)silyl]ethynyl]phenyl]-3-hexene-1,5-diyn-1-yl]-7-[(3E)-3-propyl-4-[2-[4-[2-[tris(1-methylethyl)silyl]ethynyl]phenyl]ethynyl]-3-hepten-1-yn-1-yl]- (CA INDEX NAME)

Double bond geometry as shown.

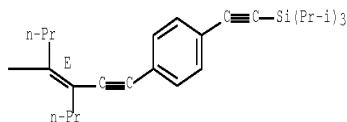


RN 864684-29-7 CAPLUS



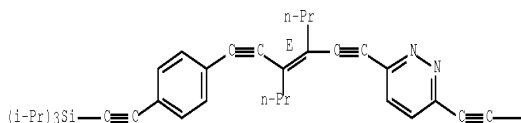
CN Pyridazine, 3-[(3E)-3,4-dipropyl-6-[4-[2-[tris(1-methylethyl)silyl]ethynyl]phenyl]-3-hexene-1,5-diyn-1-yl]-6-[(3E)-3-propyl-4-[2-[4-[2-[tris(1-methylethyl)silyl]ethynyl]phenyl]ethynyl]-3-hepten-1-yn-1-yl]- (CA INDEX NAME)

Double bond geometry as shown.

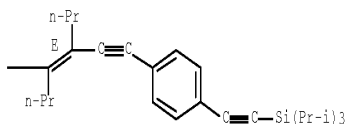


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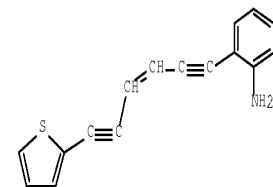
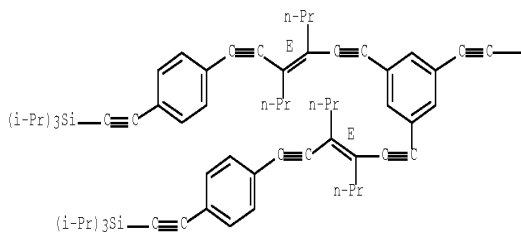


RN 864684-30-0 CAPLUS

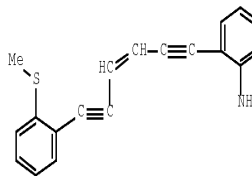
CN Benzene, 1-[(3E)-3,4-dipropyl-6-[4-[2-[tris(1-methylethyl)silyl]ethynyl]phenyl]-3-hexene-1,5-diyn-1-yl]-3-[(3E)-5-ethyl-3-propyl-4-[2-[4-[2-[tris(1-methylethyl)silyl]ethynyl]phenyl]ethynyl]-3-penten-1-yn-1-yl]-5-[(3E)-3-propyl-4-[2-[4-[2-[tris(1-methylethyl)silyl]ethynyl]phenyl]ethynyl]-3-hepten-1-yn-1-yl]- (CA INDEX NAME)

Double bond geometry as shown.

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I



II

REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L10 ANSWER 8 OF 22 CAPLUS COPYRIGHT 2009 ACS on STN  
 ACCESSION NUMBER: 2005:354187 CAPLUS [Full-text](#)  
 DOCUMENT NUMBER: 143:333  
 TITLE: Cytotoxicities, cell cycle and caspase evaluations of 1,6-diaryl-3(Z)-hexen-1,5-diynes, 2-(6-aryl-3(Z)-hexen-1,5-diynyl)anilines and their derivatives  
 AUTHOR(S): Lin, Chi-Fong; Lo, Yu-Hsiang; Hsieh, Ming-Chu; Chen, Yi-Hua; Wang, Jeh-Jeng; Wu, Ming-Jung  
 CORPORATE SOURCE: School of Chemistry, Kaohsiung Medical University, Kaohsiung, Taiwan  
 SOURCE: Bioorganic & Medicinal Chemistry (2005), 13(10), 3565-3575  
 CODEN: BMECEP; ISSN: 0968-0896  
 PUBLISHER: Elsevier Ltd.  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 OTHER SOURCE(S): CASREACT 143:333  
 GI

AB A series of compds. showed growth inhibition effects on a full panel of 60 human cancer cell lines, and most of the average IC50 values of the indicated



analogs were from <0.01 to 96.6  $\mu$ M, in which a 2-thienyl analog and the thioanisole analog revealed the highest cytotoxic activity with the cancer cell lines at 10-7M concentration range. During the cell cycle anal., a moderate to high apoptotic progress induction was shown by several compared with the control, which 2-(6-(2-thienyl)-3(Z)-hexen-1,5-diynyl)aniline (I) showed the highest apoptotic effect. I and the thioanisole analog displayed a significant G2/M phase arrest in the cell growth cycle compared with other derivs., which the proportions of the G2/M phase cells were accumulated to 71.5% and 82.6%, resp. Moreover, the colorimetric assay of the I and the thioanisole analog also provided advanced evidence to the relationship between the compds. and the caspase-3 enzyme, which was one of the major promoters of apoptotic effect.

IT 852619-13-7F

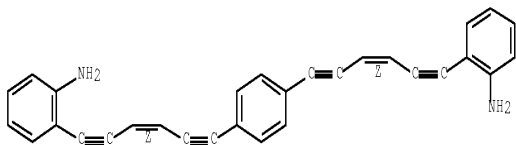
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)

(cytotoxicities, cell cycle and caspase evaluations of  
1,6-diaryl-3(Z)-hexen-1,5-diyne,  
2-(6-aryl-3(Z)-hexen-1,5-diynyl)anilines and their derivs.)

RN 852619-13-7 CAPLUS

CN Benzenamine, 2,2'-[1,4-phenylenedi-(3Z)-3-hexene-1,5-diyne-6,1-diyl]bis-(9CI) (CA INDEX NAME)

Double bond geometry as shown.



OS.CITING REF COUNT: 15 THERE ARE 15 CAPLUS RECORDS THAT CITE THIS RECORD (15 CITINGS)  
REFERENCE COUNT: 35 THERE ARE 35 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L10 ANSWER 9 OF 22 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 2005:34387 CAPLUS [Full-text](#)

DOCUMENT NUMBER: 142:135171

TITLE: Liquid crystalline compound having perfluoroalkyl side chains, liquid crystal composition containing these compounds and their polymers

INVENTOR(S): Sasada, Yasuyuki; Yanai, Motoki

PATENT ASSIGNEE(S): Chisso Petrochemical Corporation, Japan; Chisso Corporation

SOURCE: U.S. Pat. Appl. Publ., 56 pp.

CODEN: USXXCO

DOCUMENT TYPE: Patent

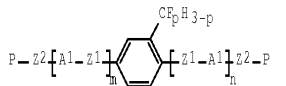
LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 20050007541	A1	20050113	US 2004-873280	20040623
US 7070838	B2	20060704		

JP 2005035985 A 20050210 JP 2004-183449 20040622  
PRIORITY APPLN. INFO.: JP 2003-177672 A 20030623  
OTHER SOURCE(S): MARPAT 142:135171  
GI



AB Liquid crystalline compds. I [P = CX22: CX1CO2, Q1, CX22: CX2O, p-CX22: CX2COC6H4, or Q2; A1 = 1,4-cyclohexenylen, 1,4-phenylene, naphthalene-2,6-diyl, tetrahydronaphthalene-2,6-diyl, fluorene-2,7-diyl, or bicyclo[2.2.2]octane-1,4-diyl, where any CH2 of these rings is optionally replaced by O, any CH: is optionally replaced by N; and any H is optionally replaced by halo, C1-5 alkyl, or halogenated alkyl; Z1 = single bond, CH2CH2, CF2CF2, (CH2)4, CH2O, OCH2, CO2, OCO, CH:CH, CF:CF, C.tplbond.C, C.tplbond.CO2, OCOC.tplbond.C, CH:CHCO2, OCOCH:CH, CH2CH2CO2, OCOCCH2CH2, C.tplbond.CCH:CH, CH:CHC.tplbond.C, OCF2, or CF2; Z2 = single bond or C1-20 alkylene, where any CH2 is optionally replaced by O, S, CO2, or OCO; X1 = H, halo, CF3 or C1-5 alkyl, X2 = H, halo, or C1-5 alkyl; m, n = 0-2; m + n  $\leq$  4; p = 2 or 3; q = 0 or 1; when Z1 is C.tplbond.C, P = Q1, CX22: CX2O, p-CX22: CX2COC6H4] are prepared The invention further provides for polymerization of a composition containing Z1 of I to give a film, an optical anisotropic material, a 1/4 or 1/2 wavelength functional plate, an optical compensation element, an optical element or a liquid crystal display element. A typical liquid crystalline compound (II) was manufactured by esterification of 2-(trifluoromethyl)-1,4-dihydroxybenzene with 4-[(6-(acryloyloxy)hexyloxy)benzoic acid in THF in the presence of 4-dimethylaminopyridine and 1-ethyl-3-(3-dimethylaminopropyl)carbodiimide overnight. A typical liquid crystalline polymer was manufactured by photopolym. of 80 parts II in a mixture containing 4-(trans-4-propylcyclohexyl)cyanobenzene 5, 4-(trans-4-pentylcyclohexyl)cyanobenzene 5, 4-(trans-4-heptylcyclohexyl)cyanobenzene 5, and 4'-(trans-4-heptylcyclohexyl)-4-cyano-1,1'-biphenyl 5 parts in the presence of Irgacure 907 as a film on a polyimide alignment film attached to a glass substrate.

IT 1056056-84-8

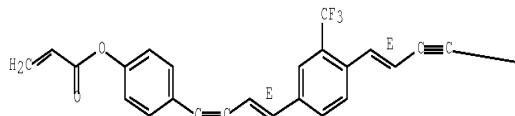
RL: PRPH (Prophetic)

(Liquid crystalline compound having perfluoroalkyl side chains, liquid crystal composition containing these compounds and their polymers)

RN 1056056-84-8 CAPLUS

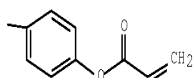
CN INDEX NAME NOT YET ASSIGNED

Double bond geometry as shown.



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OS.CITING REF COUNT: 3 THERE ARE 3 CAPLUS RECORDS THAT CITE THIS RECORD  
(3 CITINGS)

L10 ANSWER 10 OF 22 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 2004:566840 CAPLUS [Full-text](#)

DOCUMENT NUMBER: 141:261152

TITLE:  $\pi$ -Conjugated Dendrimers Based on  
Bis(enediynyl)benzene Units

AUTHOR(S): Hwang, Gil Tae; Kim, Byeang Hyeon

CORPORATE SOURCE: National Research Laboratory, Department of Chemistry,  
Division of Molecular and Life Sciences, Pohang  
University of Science and Technology, Pohang, 790-784,  
S. Korea

SOURCE: Organic Letters (2004), 6(16), 2669-2672

CODEN: ORLEF7; ISSN: 1523-7060

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

AB We have synthesized a new family of  $\pi$ -conjugated dendrimers that are based on bis(enediynyl)benzene units by using both divergent and convergent approaches. The compds. at all three generations have strong bluish-green fluorescence, especially the third-generation dendrimer, which has the highest extinction coefficient and quantum efficiency in this series.

IT 754233-15-3P 754233-16-4P 754233-17-5P

754233-13-6P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT  
(Reactant or reagent)

(convergent and divergent synthesis of  $\pi$ -conjugated dendrimers based  
on bis(enediynyl)benzene units)

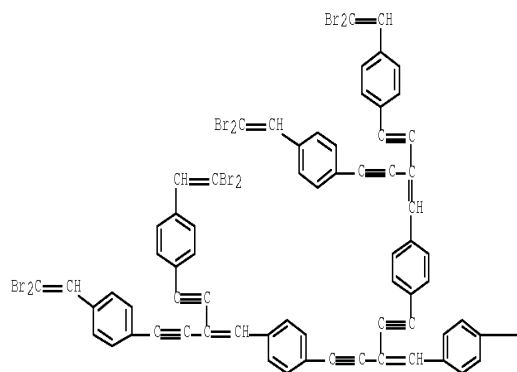
RN 754233-15-3 CAPLUS

CN Benzene, 1,4-bis[4-[4-(2,2-dibromoethenyl)phenyl]-2-[[4-(2,2-dibromoethenyl)phenyl]ethynyl]-1-buten-3-ynyl]- (9CI) (CA INDEX NAME)

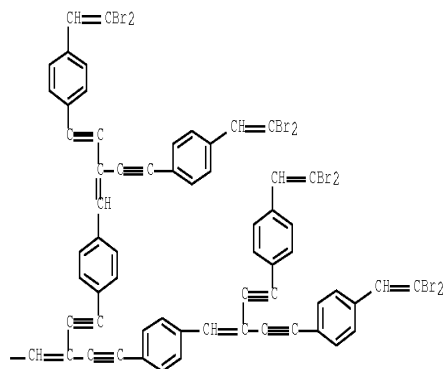
RN 754233-16-4 CAPLUS

CN Benzene, 1,4-bis[4-[4-[4-(2,2-dibromoethenyl)phenyl]-2-[[4-(2,2-dibromoethenyl)phenyl]ethynyl]-1-buten-3-ynyl]phenyl]-2-[[4-[4-(2,2-dibromoethenyl)phenyl]-2-[[4-(2,2-dibromoethenyl)phenyl]ethynyl]-1-buten-3-ynyl]phenyl]ethynyl]-1-buten-3-ynyl]- (9CI) (CA INDEX NAME)

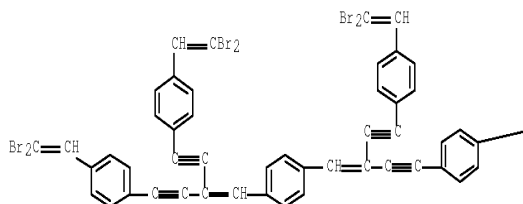
PAGE 1-A



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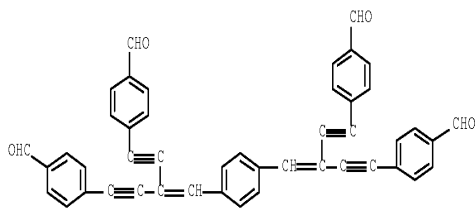
PAGE 1-A





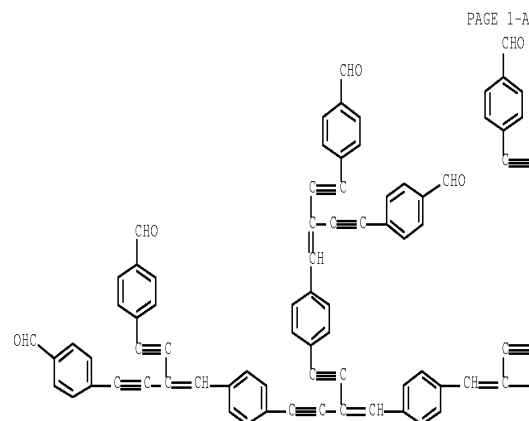
RN 754233-17-5 CAPLUS

CN Benzaldehyde, 4,4'-[[3-[[4-[4-(4-formylphenyl)-2-[(4-formylphenyl)ethynyl]-1-buten-3-ynyl]phenyl]methylene]-1,4-pentadiyne-1,5-diyl]bis- (9CI) (CA INDEX NAME)

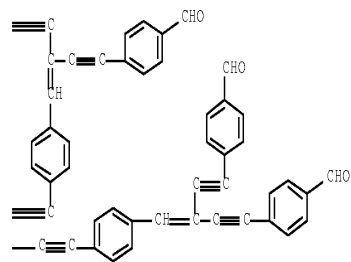


RN 754233-18-6 CAPLUS

CN Benzaldehyde, 4,4'-[[3-[[4-[4-[4-(4-formylphenyl)-2-[(4-formylphenyl)ethynyl]-1-buten-3-ynyl]phenyl]-2-[[4-[4-(4-formylphenyl)-2-[(4-formylphenyl)ethynyl]-1-buten-3-ynyl]phenyl]ethynyl]-1-buten-3-ynyl]phenyl]methylene]-1,4-pentadiyne-1,5-diyl]bis[4,1-phenylene[3-[(4-formylphenyl)ethynyl]-3-buten-1-yn-4,1-diyl]]bis- (9CI) (CA INDEX NAME)



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OS.CITING REF COUNT: 17 THERE ARE 17 CAPLUS RECORDS THAT CITE THIS RECORD (17 CITINGS)

REFERENCE COUNT: 33 THERE ARE 33 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L10 ANSWER 11 OF 22 CAPLUS COPYRIGHT 2009 ACS ON STN

ACCESSION NUMBER: 2004:480115 CAPLUS [Full-text](#)

DOCUMENT NUMBER: 141:190674

TITLE: Synthesis of Conjugated Oligomers Having Aromatic and Eneidyne Units Alternately in the Backbone that Show Intense Fluorescence Emission

AUTHOR(S): Nakano, Yuuki; Ishizuka, Kenichi; Muraoka, Kenji; Ohtani, Hiroyuki; Takayama, Yuuki; Sato, Fumie

CORPORATE SOURCE: Department of Biomolecular Engineering, Tokyo Institute of Technology, Midori, Yokohama, Kanagawa, 226-8501, Japan

SOURCE: Organic Letters (2004), 6(14), 2373-2376  
CODEN: ORLEF7; ISSN: 1523-7060

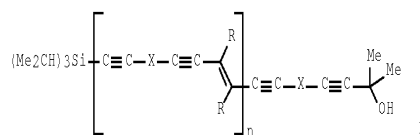
PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 141:190674

GI



AB Synthesis and fluorescence properties of  $\pi$ -conjugated compds. I ( $n = 1 - 3$ ; X = 1,4-phenylene, 2,5-pyridine, 2,5-thiophene; R = n-Pr, n-Bu) having



alternately an aromatic or heteroarom. ring and an enediyne unit in the backbone are described.

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IT 740810-62-2P 740810-65-5P 740810-68-8P

RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

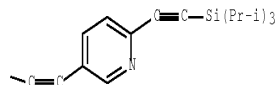
(preparation and absorption and fluorescence spectra of conjugated oligomers

having aromatic (or heteroarom.) and enediyne units alternately in the backbone)

RN 740810-62-2 CAPLUS

CN 3-Butyn-2-ol, 2-methyl-4-[4-[(3E)-3-propyl-4-[[4-[(3E)-3-propyl-4-[[4-[[tris(1-methylethyl)silyl]ethynyl]phenyl]ethynyl]-3-hepten-1-yn-1-yl]phenyl]ethynyl]-3-hepten-1-yn-1-yl]phenyl]- (CA INDEX NAME)

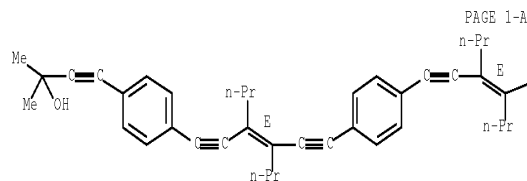
Double bond geometry as shown.



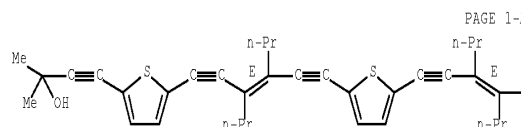
RN 740810-68-8 CAPLUS

CN 3-Butyn-2-ol, 2-methyl-4-[5-[(3E)-3-propyl-4-[[5-[(3E)-3-propyl-4-[[5-[[tris(1-methylethyl)silyl]ethynyl]-2-thienyl]ethynyl]-3-hepten-1-yn-1-yl]-2-thienyl]ethynyl]-3-hepten-1-yn-1-yl]-2-thienyl]- (CA INDEX NAME)

Double bond geometry as shown.

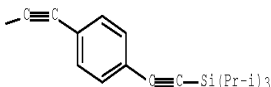


PAGE 1-A

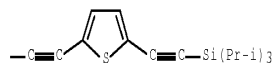


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RN 740810-65-5 CAPLUS

CN 3-Butyn-2-ol, 4-[6-[(3E)-3-butyl-4-[2-[6-[(3E)-3-butyl-4-[2-[6-[2-[tris(1-methylethyl)silyl]ethynyl]-3-pyridinyl]ethynyl]-3-hepten-1-yn-1-yl]-3-pyridinyl]ethynyl]-3-hepten-1-yn-1-yl]-3-pyridinyl]-2-methyl- (CA INDEX NAME)

Double bond geometry as shown.

IT 740810-63-3P 740810-66-6P 740810-69-9P

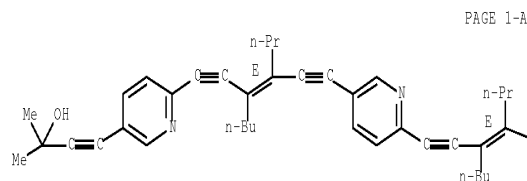
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation) (preparation and absorption and fluorescence spectra of conjugated

oligomers having aromatic (or heteroarom.) and enediyne units alternately in the backbone)

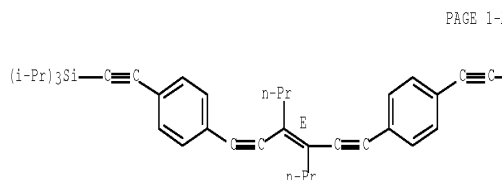
RN 740810-63-3 CAPLUS

CN 3-Butyn-2-ol, 2-methyl-4-[4-[(3E)-3-propyl-4-[[4-[(3E)-3-propyl-4-[[4-[(3E)-3-propyl-4-[[4-[[tris(1-methylethyl)silyl]ethynyl]phenyl]ethynyl]-3-hepten-1-yn-1-yl]phenyl]ethynyl]-3-hepten-1-yn-1-yl]phenyl]ethynyl]-3-hepten-1-yn-1-yl]phenyl]- (CA INDEX NAME)

Double bond geometry as shown.



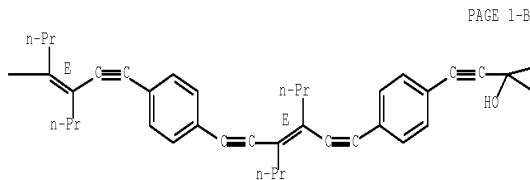
PAGE 1-A



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RN 740810-69-9 CAPLUS

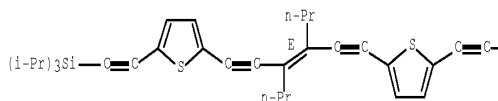
CN 3-Butyn-2-ol, 4-[5-[(3E)-4-[2-[5-[(3E)-5-ethyl-4-[2-[5-[(3E)-5-ethyl-3-propyl-4-[2-[5-[2-[tris(1-methylethyl)silyl]ethynyl]-2-thienyl]ethynyl]-3-penten-1-yn-1-yl]-2-thienyl]ethynyl]-3-propyl-3-penten-1-yn-1-yl]-2-thienyl]ethynyl]-3-propyl-3-hepten-1-yn-1-yl]-2-thienyl]-2-methyl- (CA INDEX NAME)

Double bond geometry as shown.

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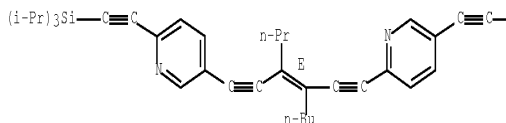


RN 740810-66-6 CAPLUS

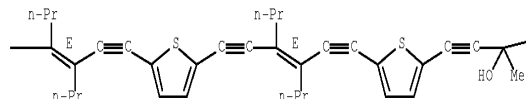
CN 3-Butyn-2-ol, 4-[6-[(3E)-3-butyl-4-[2-[6-[(3E)-3-butyl-4-[2-[6-[(3E)-3-butyl-4-[2-[6-[2-[tris(1-methylethyl)silyl]ethynyl]-3-pyridinyl]ethynyl]-3-hepten-1-yn-1-yl]-3-pyridinyl]ethynyl]-3-hepten-1-yn-1-yl]-3-pyridinyl]ethynyl]-3-hepten-1-yn-1-yl]-3-pyridinyl]ethynyl]-2-methyl- (CA INDEX NAME)

Double bond geometry as shown.

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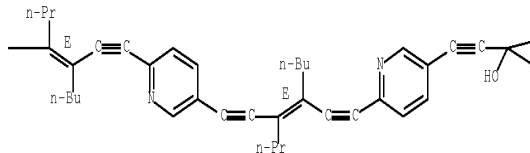
PAGE 1-B



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OS.CITING REF COUNT: 20 THERE ARE 20 CAPLUS RECORDS THAT CITE THIS RECORD (20 CITINGS)

REFERENCE COUNT: 12 THERE ARE 12 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L10 ANSWER 12 OF 22 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 2004:328526 CAPLUS [Full-text](#)

DOCUMENT NUMBER: 141:54000

TITLE: Solid-phase synthesis of oligo(triacetylene)s and oligo(phenylenetriacetylene)s employing Sonogashira and Cadiot-Chodkiewicz-type cross-coupling reactions

AUTHOR(S): Utesch, Nils F.; Diederich, Francois; Boudon, Corinne; Gisselbrecht, Jean-Paul; Gross, Maurice



CORPORATE SOURCE: Laboratorium fuer Organische Chemie, ETH-Hoenggerberg,  
HCl, Zurich, CH-8093, Switz.  
SOURCE: Helvetica Chimica Acta (2004), 87(3), 698-718  
CODEN: HCACAV; ISSN: 0018-019X  
PUBLISHER: Verlag Helvetica Chimica Acta  
DOCUMENT TYPE: Journal  
LANGUAGE: English  
OTHER SOURCE(S): CASREACT 141:54000

PAGE 1-A

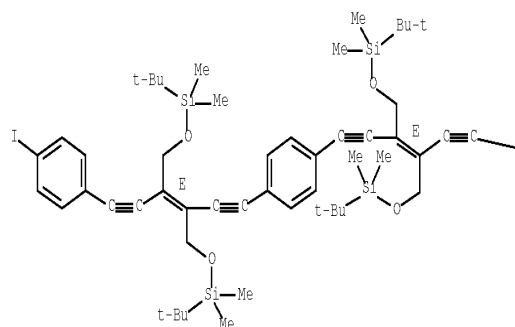
AB The polymer-supported synthesis of poly(triacetylene)-derived monodisperse oligomers is described, using Pd0-catalyzed Sonogashira and Cadiot-Chodkiewicz-type cross-couplings as the key steps in the construction of the acetylenic scaffolds. Merrifield resin functionalized with a 1-(4-iodoaryl)triazene linker was chosen as the polymeric support. The linker selection was made based on the results of several model studies in the liquid phase. For the solid-support synthesis of p-I[C6H4C.tplbond.CC(CH2OSiMe2CMe3):C(CH2OSiMe2CMe3)C.tplbond.C]nSiMe3 [I, n = 2-4] a set of only three reactions was required: (i) Pd0-catalyzed Sonogashira cross-coupling, (ii) Me3Si-alkyne deprotection by protodesilylation, and (iii) cleavage of the linker with liberation of I. The longest-wavelength absorption maxima of I [n = 1-4] shift bathochromically with increasing oligomeric length, from  $\lambda_{\text{max}}$  337 nm (I, n = 1) to 384 nm (I, n = 4). Based on the electronic absorption data, the effective conjugation length (ECL) of the oligo(phenylene triacetylene)s is estimated to involve at least four monomer units and 40 C-atoms.  $\pi$ -Electron conjugation in these oligomers is less efficient than in Me3Si[C6H4C.tplbond.CC(CH2OSiMe2CMe3):C(CH2OSiMe2CMe3)C.tplbond.C]nSiMe3 (II) due to poor transmittance of  $\pi$ -electron delocalization by the Ph rings inserted into the oligomeric backbone. Similar conclusions were drawn from the electrochem. properties of the two oligomeric series as determined by cyclic (CV) and rotating-disk voltammetry. In sharp contrast to II, I are strongly fluorescent, with the highest quantum yield  $\Phi_F$  = 0.69 measured for I [n = 3]. Whereas the Sonogashira cross-coupling on solid support proceeded smoothly, optimal conditions for alkyne-alkyne cross-coupling reactions employing Pd0-catalyzed Cadiot-Chodkiewicz conditions still remain to be developed.

IT 554453-63-1P 554459-64-2P  
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)  
(solid-phase synthesis of oligo(triacetylene)s and  
oligo(phenylenetriacetylene)s by Sonogashira and Cadiot-Chodkiewicz  
cross-coupling reactions)

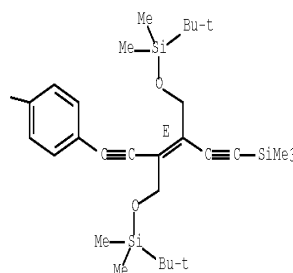
RN 554459-63-1 CAPLUS

CN 4,9-Dioxa-3,10-disiladodec-6-ene, 6-[[4-[(3E)-6-[4-[(3E)-3,4-bis[[[(1,1-dimethylethyl)dimethylsilyl]oxy]methyl]-6-(4-iodophenyl)-3-hexene-1,5-diynyl]phenyl]-3,4-bis[[[(1,1-dimethylethyl)dimethylsilyl]oxy]methyl]-3-hexene-1,5-diynyl]phenyl]ethynyl]-2,2,3,3,10,10,11,11-octamethyl-7-[(trimethylsilyl)ethynyl]-, (6E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



PAGE 1-B

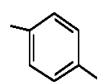
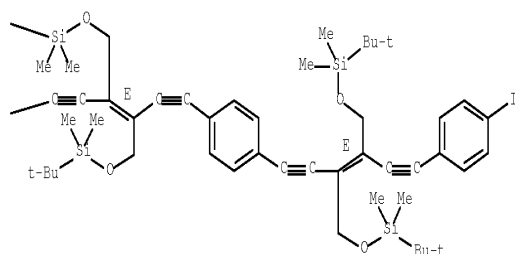
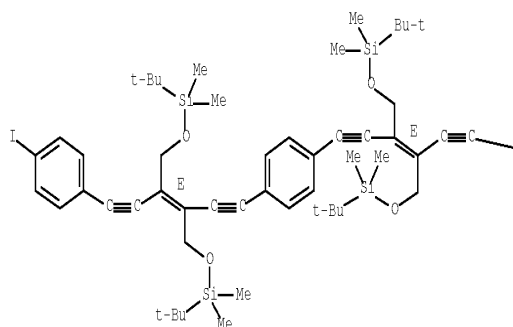
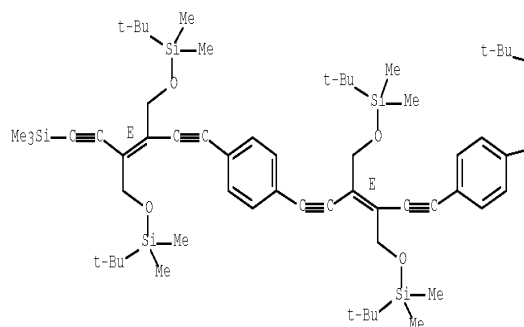


RN 554459-64-2 CAPLUS

CN 4,9-Dioxa-3,10-disiladodec-6-ene, 6-[[4-[(3E)-6-[4-[(3E)-3,4-bis[[[(1,1-dimethylethyl)dimethylsilyl]oxy]methyl]-6-(4-iodophenyl)-3-hexene-1,5-diynyl]phenyl]-3,4-bis[[[(1,1-dimethylethyl)dimethylsilyl]oxy]methyl]-3-hexene-1,5-diynyl]phenyl]ethynyl]-7-[[4-[(3E)-3,4-bis[[[(1,1-dimethylethyl)dimethylsilyl]oxy]methyl]-6-(trimethylsilyl)-3-hexene-1,5-diynyl]phenyl]ethynyl]-2,2,3,3,10,10,11,11-octamethyl-, (6E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.





IT 704916-29-0F

RL: SPN (Synthetic preparation); PREP (Preparation)  
 (solid-phase synthesis of oligo(triacetylene)s and  
 oligo(phenylenetriacetylene)s by Sonogashira and Cadiot-Chodkiewicz  
 cross-coupling reactions)

RN 704916-29-0 CAPLUS

CN 4,9-Dioxa-3,10-disiladodec-6-ene, 6,6'-(1,4-phenylenedi-2,1-  
 ethynediyl)bis[7-[(4-iodophenyl)ethynyl]-2,2,3,3,10,10,11,11-octamethyl-  
 (6E,6'E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

OS.CITING REF COUNT: 6 THERE ARE 6 CAPLUS RECORDS THAT CITE THIS RECORD  
 (6 CITINGS)

REFERENCE COUNT: 93 THERE ARE 93 CITED REFERENCES AVAILABLE FOR THIS  
 RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L10 ANSWER 13 OF 22 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 2003:827385 CAPLUS [Full-text](#)

DOCUMENT NUMBER: 140:59755

TITLE: Synthesis and reactivity of dinuclear rhodium  
 complexes with Rh:C:CHR and Rh:C:C:CRR' units as  
 building blocks

AUTHOR(S): Callejas-Gaspar, Berta; Laubender, Matthias; Werner,  
 Helmut

CORPORATE SOURCE: Institut fuer Anorganische Chemie der Universitaet  
 Wuerzburg, Wuerzburg, D-97074, Germany

SOURCE: Journal of Organometallic Chemistry (2003), 684(1-2),  
 144-152

CODEN: JORCAI; ISSN: 0022-328X

PUBLISHER: Elsevier Science B.V.

DOCUMENT TYPE: Journal

LANGUAGE: English

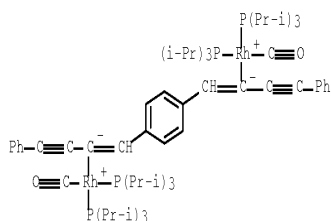
OTHER SOURCE(S): CASREACT 140:59755

AB The reaction of [Rh{κ2-O2S(O)CF3}(P4Pr3)2] (1) with ethynylferrocene in the  
 presence of KF affords the substituted vinylidene complex trans-



[RhF{C:CH(C5H4)Fe(C5H5)}(PiPr3)2] (2) which upon treatment with the butadiyne derivative Ph3SnC.tplbond.C-C.tplbond.CSnPh3 produces the chain-like compound trans-[(μ-C.tplbond.C-C.tplbond.C){Rh(:C:CH(C5H4)Fe(C5H5)}(PiPr3)2]2] (7). The triflate complex 1 reacts with 1,4-C6H4(C.tplbond.CH)2 to give the dinuclear compound trans-[(μ-1,4-C6H4(CH:C:2){Rh(η1-OS(O)2CF3)(PiPr3)2]2] (3) which in the presence of KF undergoes a ligand exchange to give the corresponding difluoro derivative trans-[(μ-1,4-C6H4(CH:C:2){RhF(PiPr3)2]2] (4). From 4 and RC.tplbond.CSnPh3 (R = CH3, C6H5) the complexes trans-[(μ-1,4-C6H4(C6H4(C6H4)2){Rh(C.tplbond.CR)(PiPr3)2]2] (5) and (6), in which a C6H4 unit bridges two alkynyl(vinylidene)rhodium(I) fragments, are obtained. Both 6 and 7 react with CO by migratory insertion of the vinylidene units into the alkynyl-metal bonds to afford the dinuclear complexes trans-[(μ-(Z,Z)-C(:CH(C5H4)Fe(C5H5)}{Rh(CO)(PiPr3)2]2] (8) and trans-[(μ-(Z,Z)-C(C.tplbond.CPh):CHC6H4CH:C(C.tplbond.CPh)}{Rh(CO)(PiPr3)2]2] (9), in which an unusual C8 or C4(C6H4)C4 chain bridges the two rhodium centers. The reactions of [RhCl(PiPr3)2]2 (10) with the functionalized diynes 1,1',4,4'-C6H4(OH)2(C.tplbond.CH)2 and 1,4-C6H4(C(Ph)(OH)C.tplbond.CH)2 lead, via the corresponding diyne-metal species (11) and (12) as intermediates, to the formation of the bis(vinylidene) complexes (13) and (14), the latter of which reacts with acidic Al2O3 by elimination of water to give the novel phenylene-bridged bis(alkenylidene)rhodium compound [(μ-1,4-C6H4(CPh:C:C:2){RhCl(PiPr3)2]2] (15) in 80% yield.

IT 639078-96-9F  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (preparation and reactivity of dinuclear rhodium carbene and alkynyl complexes)  
 RN 639078-96-9 CAPLUS  
 CN Rhodium, dicarbonyl[μ-[1,4-phenylenebis[(1Z)-1-(phenylethynyl)-2,1-ethenediyl]]]tetrakis[tris(1-methylethyl)phosphine]di-, stereoisomer (9CI)  
 (CA INDEX NAME)

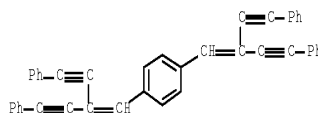


OS.CITING REF COUNT: 17 THERE ARE 17 CAPLUS RECORDS THAT CITE THIS RECORD (17 CITINGS)  
 REFERENCE COUNT: 38 THERE ARE 38 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L10 ANSWER 14 OF 22 CAPLUS COPYRIGHT 2009 ACS on STN  
 ACCESSION NUMBER: 2003:648967 CAPLUS [Full-text](#)  
 DOCUMENT NUMBER: 139:308866  
 TITLE: Synthesis and photophysical studies of bis-enediynes as tunable fluorophores  
 AUTHOR(S): Hwang, Gil Tae; Son, Hyung Su; Ku, Ja Kang; Kim, Byeang Hyeon

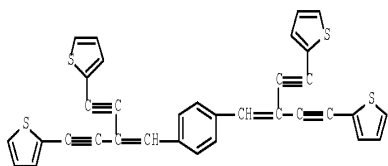
CORPORATE SOURCE: National Research Laboratory, Center for Integrated Molecular Systems, Department of Chemistry, Division of Molecular and Life Sciences, Pohang University of Science and Technology, Pohang, 790-784, S. Korea  
 SOURCE: Journal of the American Chemical Society (2003), 125(37), 11241-11248  
 CODEN: JACSAT; ISSN: 0002-7863  
 PUBLISHER: American Chemical Society  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 OTHER SOURCE(S): CASREACT 139:308866  
 AB We have synthesized a family of bis-enediynes by two complementary Pd/Cu-catalyzed Sonogashira cross-coupling methods. One is a modified Sonogashira reaction between a TMS-protected tetraalkyne and various aromatic bromides to afford bis-enediynes bearing different peripheral aryl units. The other, the reaction of bifunctional 1,1-dibromo-1-alkenes with phenylacetylene, afforded a series of bis-enediynes bearing various core aryl groups. These chemical modifications to the core and periphery of bis-enediynes induce dramatic changes in absorption and emission spectra. Bis-enediynes with peripheral aryl groups show a large Stokes shift of about 50-110 nm when compared to the less-conjugated TMS-protected bis-enediynes. Absorptions and emissions of other bis-enediynes were red-shifted relative to those of (4-phenyl-2-phenylethynyl-1-buten-3-ynyl)benzene. Substantial increases in fluorescence quantum yields are observed as a result of extending the π-conjugation. The emission wavelength of the bis-enediynes was tailored from indigo blue to reddish-orange, suggesting that the color of emission can be tunable by modification of the core and/or peripheral units.

IT 360549-89-9F 360549-90-2F 360549-91-3F  
 360549-92-4F 360549-93-5F 360549-94-6F  
 360549-95-7F 360549-96-8F 360549-97-9F  
 360549-98-0F 610283-06-2F 610283-08-4F  
 610283-09-5F 610283-10-3F 610283-11-3F  
 610283-12-0F 610283-13-1F  
 RL: PRP (Properties); SPN (Synthetic preparation); TEM (Technical or engineered material use); PREP (Preparation); USES (Uses)  
 (dye; preparation and photophys. properties of bis-enediynes as tunable fluorophores)  
 RN 360549-89-9 CAPLUS  
 CN Benzene, 1,4-bis[4-phenyl-2-(2-phenylethynyl)-1-buten-3-yn-1-yl]- (CA INDEX NAME)



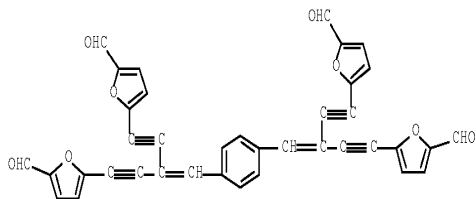
RN 360549-90-2 CAPLUS  
 CN Thiophene, 2,2'-[1,4-phenylenebis[3-(2-thienylethynyl)-3-buten-1-yn-4,1-diyl]]bis- (9CI) (CA INDEX NAME)





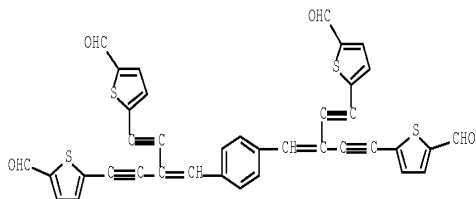
RN 360549-91-3 CAPLUS

CN 2-Furancarboxaldehyde, 5,5'-[1,4-phenylenebis[3-[(5-formyl-2-furanyl)ethynyl]-3-buten-1-yne-4,1-diyl]]bis- (9CI) (CA INDEX NAME)



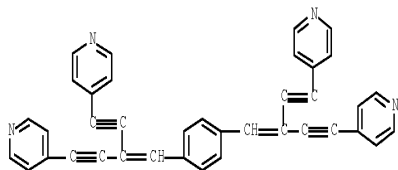
RN 360549-92-4 CAPLUS

CN 2-Thiophenecarboxaldehyde, 5,5'-[1,4-phenylenebis[3-[(5-formyl-2-thienyl)ethynyl]-3-buten-1-yne-4,1-diyl]]bis- (9CI) (CA INDEX NAME)



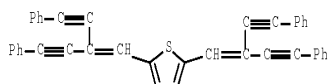
RN 360549-93-5 CAPLUS

CN Pyridine, 4,4'-[1,4-phenylenebis[3-(4-pyridinylethynyl)-3-buten-1-yne-4,1-diyl]]bis- (9CI) (CA INDEX NAME)



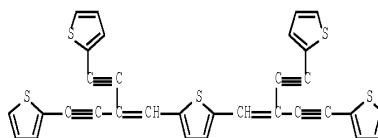
RN 360549-94-6 CAPLUS

CN Thiophene, 2,5-bis[4-phenyl-2-(2-phenylethynyl)-1-buten-3-yn-1-yl]- (CA INDEX NAME)



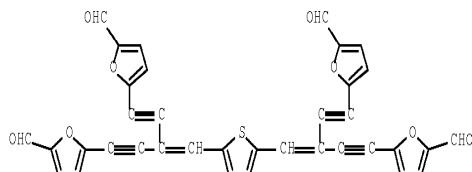
RN 360549-95-7 CAPLUS

CN Thiophene, 2,5-bis[4-(2-thienyl)-2-(2-(2-thienyl)ethynyl)-1-buten-3-yn-1-yl]- (CA INDEX NAME)



RN 360549-96-8 CAPLUS

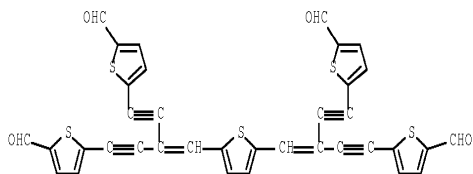
CN 2-Furancarboxaldehyde, 5,5'-[2,5-thiophenediylbis[3-[(5-formyl-2-furanyl)ethynyl]-3-buten-1-yne-4,1-diyl]]bis- (9CI) (CA INDEX NAME)



RN 360549-97-9 CAPLUS

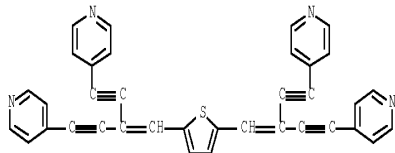
CN 2-Thiophenecarboxaldehyde, 5,5'-[2,5-thiophenediylbis[3-[(5-formyl-2-thienyl)ethynyl]-3-buten-1-yne-4,1-diyl]]bis- (9CI) (CA INDEX NAME)





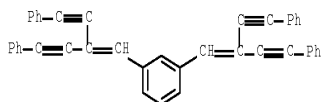
RN 360549-98-0 CAPLUS

CN Pyridine, 4,4'-[2,5-thiophenediylbis[3-(4-pyridinylethynyl)-3-buten-1-yn-4,1-diyl]]bis- (9CI) (CA INDEX NAME)



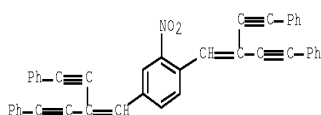
RN 610283-06-2 CAPLUS

CN Benzene, 1,3-bis[4-phenyl-2-(2-phenylethynyl)-1-buten-3-yn-1-yl]- (CA INDEX NAME)



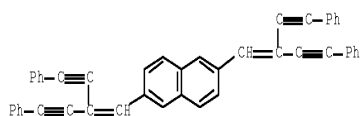
RN 610283-08-4 CAPLUS

CN Benzene, 2-nitro-1,4-bis[4-phenyl-2-(2-phenylethynyl)-1-buten-3-yn-1-yl]- (CA INDEX NAME)



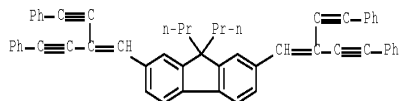
RN 610283-09-5 CAPLUS

CN Naphthalene, 2,6-bis[4-phenyl-2-(2-phenylethynyl)-1-buten-3-yn-1-yl]- (CA INDEX NAME)



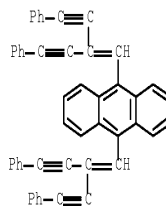
RN 610283-10-8 CAPLUS

CN 9H-Fluorene, 2,7-bis[4-phenyl-2-(2-phenylethynyl)-1-buten-3-yn-1-yl]-9,9-dipropyl- (CA INDEX NAME)



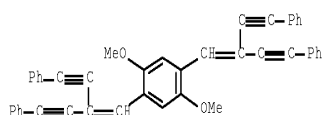
RN 610283-11-9 CAPLUS

CN Anthracene, 9,10-bis[4-phenyl-2-(2-phenylethynyl)-1-buten-3-yn-1-yl]- (CA INDEX NAME)



RN 610283-12-0 CAPLUS

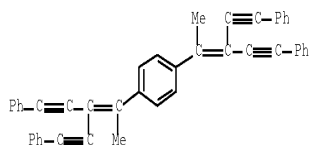
CN Benzene, 1,4-dimethoxy-2,5-bis[4-phenyl-2-(2-phenylethynyl)-1-buten-3-yn-1-yl]- (CA INDEX NAME)



RN 610283-13-1 CAPLUS

CN Benzene, 1,4-bis[1-methyl-4-phenyl-2-(2-phenylethynyl)-1-buten-3-yn-1-yl]- (CA INDEX NAME)





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OS.CITING REF COUNT: 44 THERE ARE 44 CAPLUS RECORDS THAT CITE THIS RECORD (44 CITINGS)

REFERENCE COUNT: 31 THERE ARE 31 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L10 ANSWER 15 OF 22 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 2003:424686 CAPLUS [Full-text](#)

DOCUMENT NUMBER: 139:150012

TITLE: Synthesis of Highly Fluorescent Y-Enyne Dendrimers with Four and Six Arms

AUTHOR(S): Kaafarani, Bilal R.; Wex, Brigitte; Wang, Fei; Catanescu, Otilia; Chien, L. C.; Neckers, Douglas C.

CORPORATE SOURCE: Center for Photochemical Sciences, Bowling Green State University, Bowling Green, OH, 43403, USA

SOURCE: Journal of Organic Chemistry (2003), 68(13), 5377-5380  
CODEN: JOCEAH; ISSN: 0022-3263

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

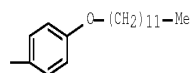
AB A first generation of dendrimeric Y-enynes with extended flexible chains was synthesized using Sonogashira coupling. Dendrimers 9 and 10 are highly fluorescent in the solid state and in solution

IT 569670-23-0P 569670-23-1P

RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)  
(synthesis of highly fluorescent Y-ene-yne dendrimers with four and six arms)

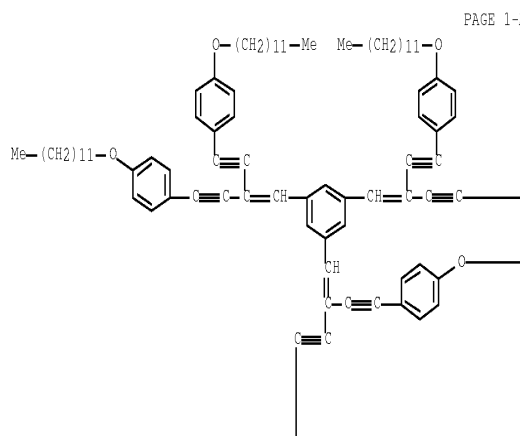
RN 569670-22-0 CAPLUS

CN Benzene, 1,4-bis[4-(4-(dodecyloxy)phenyl)-2-[[4-(dodecyloxy)phenyl]ethynyl]-1-buten-3-ynyl]- (9CI) (CA INDEX NAME)



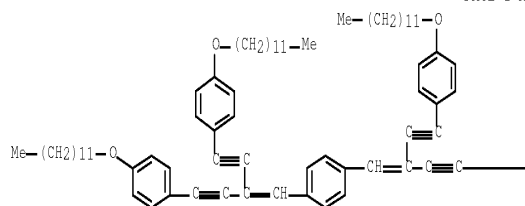
RN 569670-23-1 CAPLUS

CN Benzene, 1,3,5-tris[4-(4-(dodecyloxy)phenyl)-2-[[4-(dodecyloxy)phenyl]ethynyl]-1-buten-3-ynyl]- (9CI) (CA INDEX NAME)

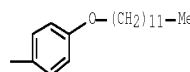


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PAGE 1-A

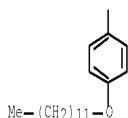


PAGE 1-B



-(CH2)11-Me





OS.CITING REF COUNT: 16 THERE ARE 16 CAPLUS RECORDS THAT CITE THIS RECORD (16 CITINGS)

REFERENCE COUNT: 41 THERE ARE 41 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L10 ANSWER 16 OF 22 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 2003:234291 CAPLUS [Full-text](#)

DOCUMENT NUMBER: 139:85055

TITLE: Acetylenic scaffolding on solid support:  
Poly(triacetylene)-derived oligomers by Sonogashira and Cadiot-Chodkiewicz-type cross-coupling reactions

AUTHOR(S): Utesch, Nils F.; Diederich, Francois

CORPORATE SOURCE: Laboratorium fur Organische Chemie, ETH-Honggerberg, HCI, Zurich, CH-8093, Switz.

SOURCE: Organic & Biomolecular Chemistry (2003), 1(2), 237-239  
CODEN: OBCRAK; ISSN: 1477-0520

PUBLISHER: Royal Society of Chemistry

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 139:85055

AB Synthesis of poly(triacetylene)-derived oligomers by Pd(0)-catalyzed Sonogashira and Cadiot-Chodkiewicz-type cross-coupling reactions on solid support is reported. Oligo(phenylene triacetylene)s, e.g., I[4-C6H4C.tplbond.CCR:CR:CR.tplbond.C]nSiMe3 (R = CH2OSiButMe2, n = 1, 2, 3, 4) members of a new class of linearly  $\pi$ -conjugated oligomers with all-C backbones, feature very high fluorescence intensities.

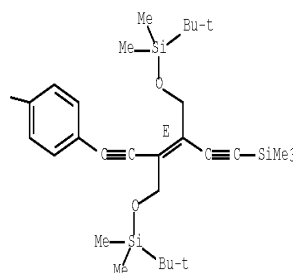
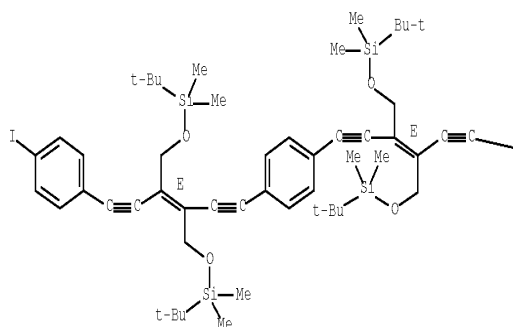
IT 554459-63-1P 554459-64-2P

RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)  
(electronic absorption and emission, UV/VIS spectra;  
poly(triacetylene)-derived oligomers are prepared by Sonogashira and Cadiot-Chodkiewicz-type Pd-catalyzed cross-coupling reactions)

RN 554459-63-1 CAPLUS

CN 4,9-Dioxa-3,10-disiladodec-6-ene, 6-[[4-[(3E)-6-[4-[(3E)-3,4-bis[[[(1,1-dimethylethyl)dimethylsilyl]oxy]methyl]-6-(4-iodophenyl)-3-hexene-1,5-diynyl]phenyl]-3,4-bis[[[(1,1-dimethylethyl)dimethylsilyl]oxy]methyl]-3-hexene-1,5-diynyl]phenyl]ethynyl]-2,2,3,3,10,10,11,11-octamethyl-7-[(trimethylsilyl)ethynyl]-, (6E)-(9CI) (CA INDEX NAME)

Double bond geometry as shown.



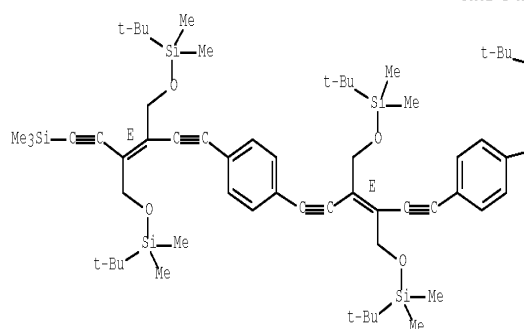
RN 554459-64-2 CAPLUS

CN 4,9-Dioxa-3,10-disiladodec-6-ene, 6-[[4-[(3E)-6-[4-[(3E)-3,4-bis[[[(1,1-dimethylethyl)dimethylsilyl]oxy]methyl]-6-(4-iodophenyl)-3-hexene-1,5-diynyl]phenyl]-3,4-bis[[[(1,1-dimethylethyl)dimethylsilyl]oxy]methyl]-3-hexene-1,5-diynyl]phenyl]ethynyl]-7-[[4-[(3E)-3,4-bis[[[(1,1-dimethylethyl)dimethylsilyl]oxy]methyl]-6-(trimethylsilyl)-3-hexene-1,5-diynyl]phenyl]ethynyl]-2,2,3,3,10,10,11,11-octamethyl-, (6E)-(9CI) (CA INDEX NAME)

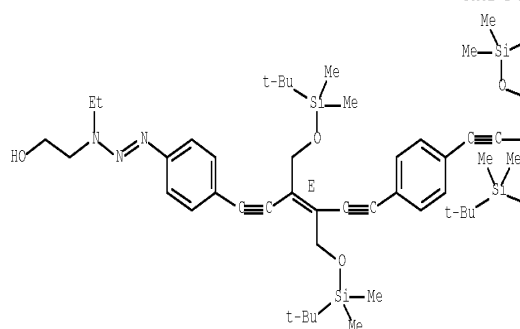
Double bond geometry as shown.



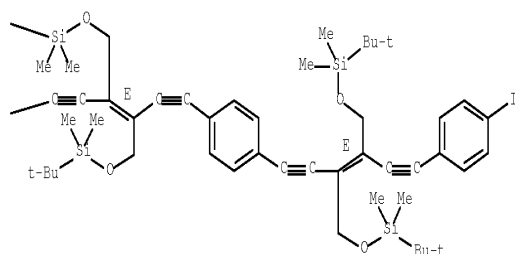
PAGE 1-A



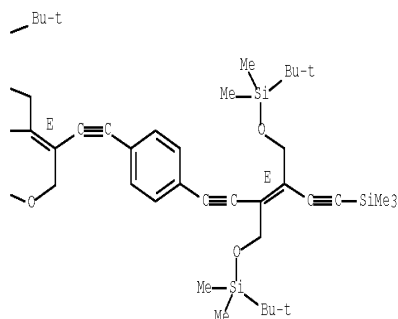
PAGE 1-A



PAGE 1-B



PAGE 1-B



IT 554459-72-2 MF, Merrifield resin-supported  
 554459-73-3 MF, Merrifield resin-supported  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT  
 (Reactant or reagent)

(preparation and Sonogashira and Cadiot-Chodkiewicz-type Pd-catalyzed  
 cross-coupling reactions of supported poly(triacetylene)-derived  
 oligomers)

RN 554459-72-2 CAPLUS

CN Ethanol, 2-[3-[4-[(3E)-6-[4-[(3E)-6-[4-[(3E)-3,4-bis[[[(1,1-dimethylethyl)dimethylsilyl]oxy]methyl]-6-(trimethylsilyl)-3-hexene-1,5-diyn-1-yl]phenyl]-3,4-bis[[[(1,1-dimethylethyl)dimethylsilyl]oxy]methyl]-3-hexene-1,5-diyn-1-yl]phenyl]-3,4-bis[[[(1,1-dimethylethyl)dimethylsilyl]oxy]methyl]-3-hexene-1,5-diyn-1-yl]phenyl]-1-ethyl-2-triazene-1-yl]- (CA INDEX NAME)

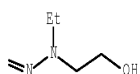
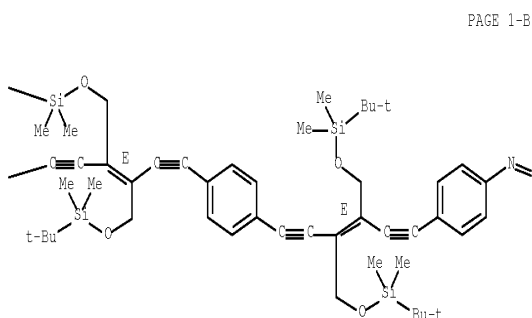
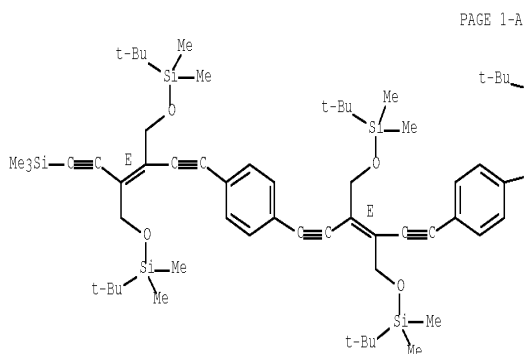
Double bond geometry as described by E or Z.

RN 554459-73-3 CAPLUS

CN Ethanol, 2-[3-[4-[(3E)-6-[4-[(3E)-6-[4-[(3E)-3,4-bis[[[(1,1-dimethylethyl)dimethylsilyl]oxy]methyl]-6-(trimethylsilyl)-3-hexene-1,5-diyn-1-yl]phenyl]-3,4-bis[[[(1,1-dimethylethyl)dimethylsilyl]oxy]methyl]-3-hexene-1,5-diyn-1-yl]phenyl]-3,4-bis[[[(1,1-dimethylethyl)dimethylsilyl]oxy]methyl]-3-hexene-1,5-diyn-1-yl]phenyl]-1-ethyl-2-triazene-1-yl]- (CA INDEX NAME)

Double bond geometry as described by E or Z.





OS.CITING REF COUNT: 18 THERE ARE 18 CAPLUS RECORDS THAT CITE THIS RECORD (18 CITINGS)

REFERENCE COUNT: 38 THERE ARE 38 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L10 ANSWER 17 OF 22 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 2001:714296 CAPLUS [Full-text](#)

DOCUMENT NUMBER: 136:69640

TITLE: Synthesis and spectroscopic studies of expanded planar dehydrotribenzo[n]annulenes containing one or two isolated alkene units

AUTHOR(S): Wan, W. Brad; Chiechi, Ryan C.; Weakley, Timothy J. R.; Haley, Michael M.

CORPORATE SOURCE: Department of Chemistry and the Materials Science Institute, University of Oregon, Eugene, OR, 97403-1253, USA

SOURCE: European Journal of Organic Chemistry (2001), (18), 3485-3490

CODEN: EJOCFK; ISSN: 1434-193X

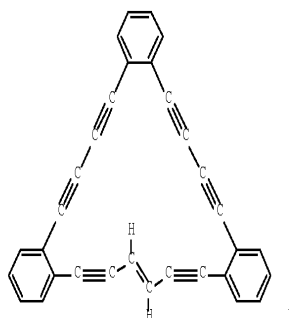
PUBLISHER: Wiley-VCH Verlag GmbH

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 136:69640

GI



AB Dehydrobenzoannulene derivs. containing isolated alkene linkages, e.g., I, were synthesized by combining an in situ Pd/Cu-mediated cross-coupling with an intramol. cyclization strategy. 1H NMR studies of these macrocycles and comparison with related systems verify that highly alkynylated dehydrobenzoannulenes possess weak induced ring currents, indicative of aromatic ( $4n+2$   $\pi$  systems) and antiarom. ( $4n$   $\pi$  systems) behavior, in spite of their large size and extensive benzannulation.

IT 363404-38-4P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

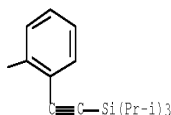
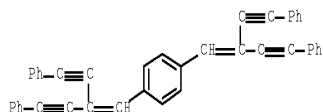
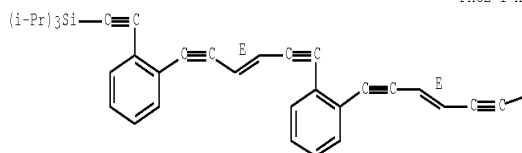
(preparation and spectroscopic studies of expanded planar dehydrotribenzo[n]annulenes containing one or two isolated alkene units)

RN 363404-38-4 CAPLUS

CN Silane, [1,2-phenylenebis[(3E)-3-hexene-1,5-diyne-6,1-diyl-2,1-phenylene-2,1-ethynediyl]]bis[tris(1-methylethyl)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.





OS.CITING REF COUNT: 10 THERE ARE 10 CAPLUS RECORDS THAT CITE THIS RECORD (10 CITINGS)

REFERENCE COUNT: 33 THERE ARE 33 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L10 ANSWER 18 OF 22 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 2001:519766 CAPLUS [Full-text](#)

DOCUMENT NUMBER: 135:243732

TITLE: Novel fluorophores: efficient synthesis and photophysical study

AUTHOR(S): Hwang, Gil Tae; Son, Hyung Su; Ku, Ja Kang; Kim, Byeang Hyeon

CORPORATE SOURCE: Center for Integrated Molecular Systems Department of Chemistry Division of Molecular Life Science, Pohang University of Science and Technology, Pohang, 790-784, S. Korea

SOURCE: Organic Letters (2001), 3(16), 2469-2471

CODEN: ORLEF7; ISSN: 1523-7060

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 135:243732

AB We have synthesized novel tetraacetylenic fluorophores by using Sonogashira reactions of 1,4-bis(dibromovinyl)benzene and 2,5-bis(dibromovinyl)thiophene with various aromatic bromides. The emission maxima of these fluorophores vary from the indigo blue to the reddish-orange region, depending on the structures of the aromatic nuclei and peripheral moieties.

IT 360549-89-9P 360549-90-2P 360549-91-3P

360549-92-4P 360549-93-5P 360549-94-6P

360549-95-7P 360549-96-8P 360549-97-9P

360549-98-0P

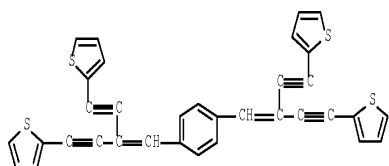
RL: PRP (Properties); SPN (Synthetic preparation); TEM (Technical or engineered material use); PREP (Preparation); USES (Uses)  
(fluorescent dye; preparation and spectra of tetraacetylenic fluorophores)

RN 360549-89-9 CAPLUS

CN Benzene, 1,4-bis[4-phenyl-2-(2-phenylethynyl)-1-buten-3-yn-1-yl]- (CA

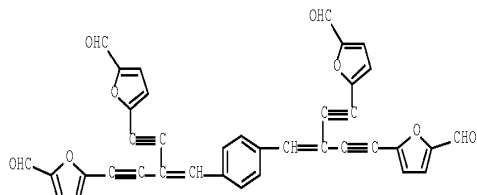
RN 360549-90-2 CAPLUS

CN Thiophene, 2,2'-[1,4-phenylenebis[3-(2-thienylethynyl)-3-buten-1-yn-4,1-diyl]]bis- (9CI) (CA INDEX NAME)



RN 360549-91-3 CAPLUS

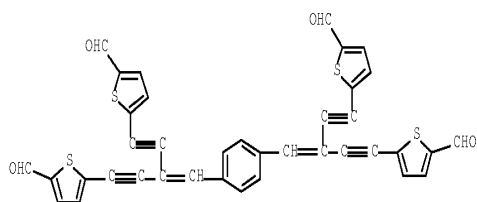
CN 2-Furancarboxaldehyde, 5,5'-[1,4-phenylenebis[3-[(5-formyl-2-furanyl)ethynyl]-3-buten-1-yn-4,1-diyl]]bis- (9CI) (CA INDEX NAME)



RN 360549-92-4 CAPLUS

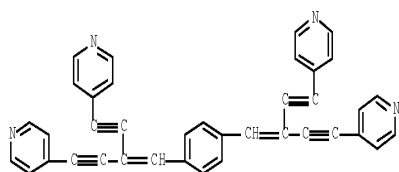
CN 2-Thiophenecarboxaldehyde, 5,5'-[1,4-phenylenebis[3-[(5-formyl-2-thienyl)ethynyl]-3-buten-1-yn-4,1-diyl]]bis- (9CI) (CA INDEX NAME)





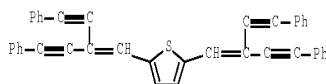
RN 360549-93-5 CAPLUS

CN Pyridine, 4,4'-[1,4-phenylenebis[3-(4-pyridinylethynyl)-3-buten-1-yne-4,1-diyl]]bis- (9CI) (CA INDEX NAME)



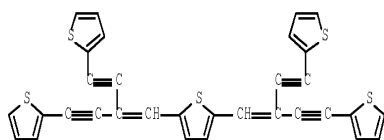
RN 360549-94-6 CAPLUS

CN Thiophene, 2,5-bis[4-(2-thienyl)-2-(2-phenylethynyl)-1-buten-3-yn-1-yl]- (CA INDEX NAME)



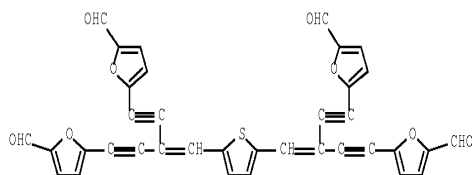
RN 360549-95-7 CAPLUS

CN Thiophene, 2,5-bis[4-(2-thienyl)-2-(2-(2-thienyl)ethynyl)-1-buten-3-yn-1-yl]- (CA INDEX NAME)



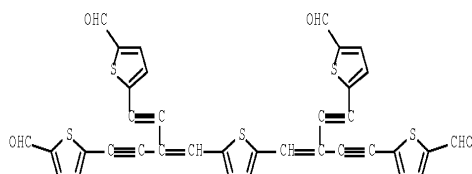
RN 360549-96-8 CAPLUS

CN 2-Furancarboxaldehyde, 5,5'-[2,5-thiophenediylbis[3-[(5-formyl-2-furanyl)ethynyl]-3-buten-1-yne-4,1-diyl]]bis- (9CI) (CA INDEX NAME)



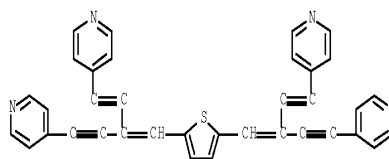
RN 360549-97-9 CAPLUS

CN 2-Thiophenecarboxaldehyde, 5,5'-[2,5-thiophenediylbis[3-[(5-formyl-2-thienyl)ethynyl]-3-buten-1-yne-4,1-diyl]]bis- (9CI) (CA INDEX NAME)



RN 360549-98-0 CAPLUS

CN Pyridine, 4,4'-[2,5-thiophenediylbis[3-(4-pyridinylethynyl)-3-buten-1-yne-4,1-diyl]]bis- (9CI) (CA INDEX NAME)



OS.CITING REF COUNT: 26 THERE ARE 26 CAPLUS RECORDS THAT CITE THIS RECORD (26 CITINGS)

REFERENCE COUNT: 20 THERE ARE 20 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L10 ANSWER 19 OF 22 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1996:29553 CAPLUS [Full-text](#)

DOCUMENT NUMBER: 124:260436

ORIGINAL REFERENCE NO.: 124:48247a,48250a

TITLE: Synthesis and reactions of new ethynyl-substituted 1,6-methano[10]annulenes

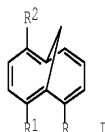
AUTHOR(S): Bryant-Freidrich, Amanda; Neidlein, Richard

CORPORATE SOURCE: Pharm.-Chem. Inst., Univ. Heidelberg, Heidelberg, D-69120, Germany

SOURCE: Synthesis (1995), (12), 1506-10

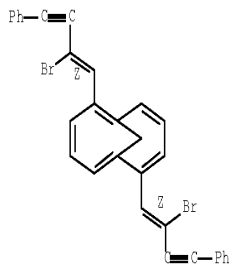


PUBLISHER: Thieme  
DOCUMENT TYPE: Journal  
LANGUAGE: English  
OTHER SOURCE(S): CASREACT 124:260436  
GI



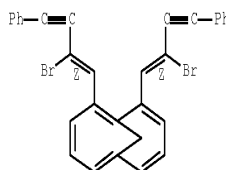
AB Stereospecific Pd(PPh<sub>3</sub>)<sub>4</sub> catalyzed coupling of an acetylene to geminal dibromo-substituted alkenes yielded enynes, which upon dehydrohalogenation formed butadiynyl substituted 1,6-methano[10]annulenes I [R = (C.tplbond.C)2R<sub>3</sub>; R<sub>1</sub> = R<sub>2</sub> = H, R<sub>3</sub> = Ph, CMe<sub>3</sub>; R<sub>1</sub> = H, R = R<sub>2</sub> = (C.tplbond.C)2Ph; R = R<sub>1</sub> = (C.tplbond.C)2Ph, R<sub>2</sub> = H].  
IT 175430-03-3P 175430-11-2P  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(preparation and reactions of ethynyl-substituted methanoannulenes)  
RN 175430-09-8 CAPLUS  
CN Bicyclo[4.4.1]undeca-1,3,5,7,9-pentaene,  
2,7-bis(2-bromo-4-phenyl-1-buten-3-ynyl)-, (Z,Z)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



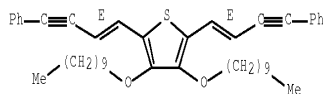
RN 175430-11-2 CAPLUS  
CN Bicyclo[4.4.1]undeca-1,3,5,7,9-pentaene,  
2,10-bis(2-bromo-4-phenyl-1-buten-3-ynyl)-, (Z,Z)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



L10 ANSWER 20 OF 22 CAPLUS COPYRIGHT 2009 ACS on STN  
ACCESSION NUMBER: 1994:192448 CAPLUS [Full-text](#)  
DOCUMENT NUMBER: 120:192448  
ORIGINAL REFERENCE NO.: 120:34087a,34090a  
TITLE: Synthesis of a series of conjugated enyne polythiophenes  
AUTHOR(S): Kane, James J.; Gao, Feng; Reinhardt, Bruce A.; Evers, Robert C.  
CORPORATE SOURCE: Chem. Dep., Wright State Univ., Dayton, OH, 45435-0001, USA  
SOURCE: Polymer Preprints (American Chemical Society, Division of Polymer Chemistry) (1992), 33(1), 1064-5  
CODEN: ACPPAY; ISSN: 0032-3934  
DOCUMENT TYPE: Journal  
LANGUAGE: English  
AB The title polymers were prepared via polymerization of 3,4-didecyloxy-2,5-bis-(β-bromoethenyl)thiophene and aromatic diethynyl compds. Thermal and viscosity of the resulting thiophene-containing polyacetylenes are discussed.  
IT 153846-90-3P  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(preparation and polymerization of, with aromatic diethynyl compds.)  
RN 153846-90-3 CAPLUS  
CN Thiophene, 3,4-bis(decyloxy)-2,5-bis(4-phenyl-1-buten-3-ynyl)-, (E,E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



OS.CITING REF COUNT: 1 THERE ARE 1 CAPLUS RECORDS THAT CITE THIS RECORD (1 CITINGS)

L10 ANSWER 21 OF 22 CAPLUS COPYRIGHT 2009 ACS on STN  
ACCESSION NUMBER: 1984:23114 CAPLUS [Full-text](#)  
DOCUMENT NUMBER: 100:23114  
ORIGINAL REFERENCE NO.: 100:3653a,3656a  
TITLE: Cis-Enyne aromatic and aromatic heterocyclic polymers  
INVENTOR(S): Reinhart, Bruce  
PATENT ASSIGNEE(S): United States Dept. of the Air Force, USA  
SOURCE: U. S. Pat. Appl., 4 pp. Avail. NTIS Order No.



PAT-APPL-6-399 661.  
 CODEN: XAXXAV  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 399661	A0	19830304	US 1982-399661	19820719
US 4417039	A	19831122		

PRIORITY APPLN. INFO.: US 1982-399661 19820719

AB Aromatic and aromatic heterocyclic enyne polymers having relatively low glass temps. for fabrication are prepared by treating 1,4-bis(cis- $\beta$ -bromovinyl)benzene (I) [88248-70-8] with a diacetylenic compound. The polymers exhibit high glass temps. and low solvent susceptibilities after heat treatment. Thus, a suspension of 40 g p-phenylenediacrylic acid [16323-43-6] in 300 g Br was stirred for 3 h to give  $\beta,\beta'$ -p-phenylenebis( $\alpha,\beta$ -dibromopropionic acid) (II) [88248-71-9]. A mixture of 21.5 g II and 20.0 g NaHCO<sub>3</sub> in 500 mL acetone was refluxed for 72 h to give I. A mixture of 0.5 g I and 0.7658 g 4,4'-bis(3-ethynylphenoxy)diphenyl sulfone [63770-82-1] was dissolved in a solution of 3 mL Et<sub>3</sub>N and 3 mL N,N-dimethylacetamide (III). A mixture of 0.025 g CuI and 0.05 g (Ph<sub>3</sub>P)<sub>2</sub>PdCl<sub>2</sub> was added. The mixture was stirred at room temperature for 70 h. Addnl. 10 mL III was added to give a polymer having glass temperature 143°. The polymer [88249-72-3] treated at 250° for 6 h had glass temperature >375° and was insol. in solvents.

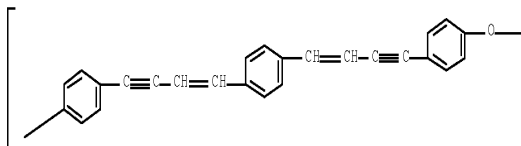
IT 88249-72-3 88249-71-9 88249-72-3

RL: IMF (Industrial manufacture); PREP (Preparation)  
 (manufacture of, with low glass temperature)

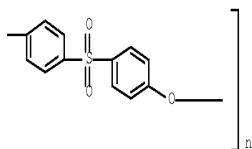
RN 88249-70-1 CAPLUS

CN Poly(oxy-1,4-phenylenesulfonyl-1,4-phenyleneoxy-1,4-phenylene-3-buten-1-yne-1,4-diyl-1,4-phenylene-1-buten-3-yne-1,4-diyl-1,4-phenylene), (Z,Z)-(9CI) (CA INDEX NAME)

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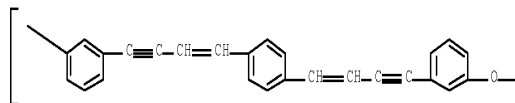


PAGE 1-B

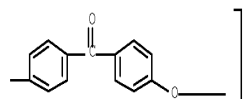


CN Poly(oxy-1,4-phenylenecarbonyl-1,4-phenyleneoxy-1,3-phenylene-3-buten-1-yne-1,4-diyl-1,4-phenylene-1-buten-3-yne-1,4-diyl-1,3-phenylene), (Z,Z)-(9CI) (CA INDEX NAME)

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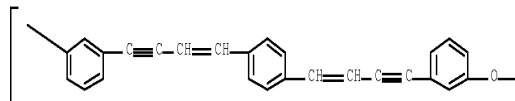
PAGE 1-B



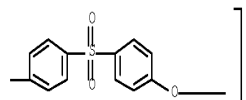
RN 88249-72-3 CAPLUS

CN Poly(oxy-1,4-phenylenesulfonyl-1,4-phenyleneoxy-1,3-phenylene-3-buten-1-yne-1,4-diyl-1,4-phenylene-1-buten-3-yne-1,4-diyl-1,3-phenylene), (Z,Z)-(9CI) (CA INDEX NAME)

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PAGE 1-B



OS.CITING REF COUNT: 4 THERE ARE 4 CAPLUS RECORDS THAT CITE THIS RECORD (4 CITINGS)

L10 ANSWER 22 OF 22 CAPLUS COPYRIGHT 2009 ACS on STN  
 ACCESSION NUMBER: 1981:175327 CAPLUS Full-text

RN 88249-71-2 CAPLUS



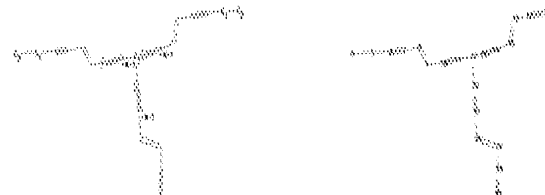
Chemical structure I: A linear polyene chain consisting of three p-phenylene rings connected by two internal double bonds. The chain is represented as: Me-C<sub>6</sub>H<sub>4</sub>-C(=CH)-C(=CH)-C<sub>6</sub>H<sub>4</sub>-C(=CH)-C(=CH)-C<sub>6</sub>H<sub>4</sub>-Me.

Chemical structure II: A cyclic polyene chain consisting of a cyclohexene ring substituted with three methyl groups, connected to a linear polyene chain that ends in a p-nitrophenyl group. The chain is represented as: Me<sub>3</sub>C<sub>6</sub>H<sub>3</sub>-C(=CH)-C(=CH)-C(=CH)-C(=CH)-C(=CH)-C<sub>6</sub>H<sub>4</sub>-NO<sub>2</sub>.

IT 77295-85-3D  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (preparation of)  
 RN 77295-85-3 CAPLUS  
 CN Benzene, 1,4-bis[4-(4-methylphenyl)-1-buten-3-ynyl]  
 INDEX NAME)

Cc1ccc(cc1)/C=C/C=C/C=C/c2ccc(cc2)/C=C/C(=O)c3ccc(C)cc3

Uploading C:\Program Files\STNEXP\Queries\10591950-cliam 3-v 1.str



2 ANSWERS

SEARCH TIME: 00.00.34



L12 2 SEA SSS FUL L11

=> file caplus

=> s l12

L13 2 L12

=> d ibib abs hitstr 1-

YOU HAVE REQUESTED DATA FROM 2 ANSWERS - CONTINUE? Y/(N):y

L13 ANSWER 1 OF 2 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 2005:1004691 CAPLUS [Full-text](#)

DOCUMENT NUMBER: 143:306181

TITLE: Process for preparation of  $\pi$ -conjugated aromatic ring-containing acetylene derivatives as organic electroluminescent devices

INVENTOR(S): Sato, Fumie; Takayama, Yuuki

PATENT ASSIGNEE(S): Nissan Chemical Industries, Ltd., Japan

SOURCE: PCT Int. Appl., 82 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

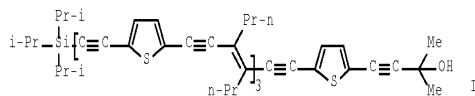
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005085176	A1	20050915	WO 2005-JP3950	20050308
W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW			
RW:	BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG			
US 20070176164	A1	20070802	US 2007-591950	20070307
PRIORITY APPLN. INFO.:			JP 2004-65446	A 20040309
			WO 2005-JP3950	W 20050308

ASSIGNMENT HISTORY FOR US PATENT AVAILABLE IN LSUS DISPLAY FORMAT

OTHER SOURCE(S): MARPAT 143:306181

GI



AB This invention pertains to a method for producing  $\pi$ -conjugated aromatic ring-containing acetylene derivs. via coupling reaction in the presence of

palladium and Cu(I) catalysts. For example, the compound I was prepared in a multi-step synthesis in good yield. The title compds. are useful as electroluminescent devices.

IT 864684-30-00

RL: DEV (Device component use); IMF (Industrial manufacture); SPN (Synthetic preparation); TEM (Technical or engineered material use); PREP (Preparation); USES (Uses)

(preparation of  $\pi$ -conjugated aromatic ring-containing acetylene derivs. as organic

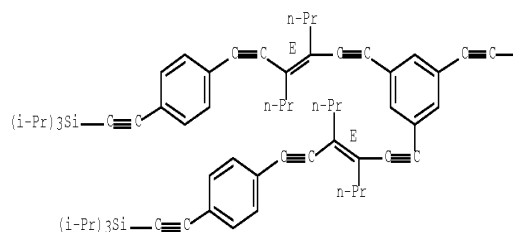
electroluminescent devices)

RN 864684-30-0 CAPLUS

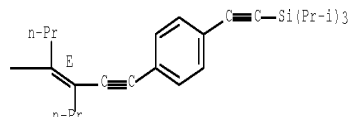
CN Benzene, 1-[(3E)-3,4-dipropyl-6-[4-[2-[tris(1-methylethyl)silyl]ethynyl]phenyl]-3-hexene-1,5-diyn-1-yl]-3-[(3E)-5-ethyl-3-propyl-4-[2-[4-[2-[tris(1-methylethyl)silyl]ethynyl]phenyl]ethynyl]-3-penten-1-yn-1-yl]-5-[(3E)-3-propyl-4-[2-[4-[2-[tris(1-methylethyl)silyl]ethynyl]phenyl]ethynyl]-3-hepten-1-yn-1-yl]- (CA INDEX NAME)

Double bond geometry as shown.

PAGE 1-A



PAGE 1-B



REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L13 ANSWER 2 OF 2 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 2003:424686 CAPLUS [Full-text](#)

DOCUMENT NUMBER: 139:150012

TITLE: Synthesis of Highly Fluorescent Y-Enyne Dendrimers with Four and Six Arms

AUTHOR(S): Kaafarani, Bilal R.; Wex, Brigitte; Wang, Fei; Catanescu, Otilia; Chien, L. C.; Neckers, Douglas C.

CORPORATE SOURCE: Center for Photochemical Sciences, Bowling Green State University, Bowling Green, OH, 43403, USA

SOURCE: Journal of Organic Chemistry (2003), 68(13), 5377-5380



PUBLISHER: American Chemical Society  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English

AB A first generation of dendrimeric Y-enynes with extended flexible chains was synthesized using Sonogashira coupling. Dendrimers 9 and 10 are highly fluorescent in the solid state and in solution

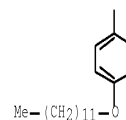
IT 569670-23-1P

RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)  
 (synthesis of highly fluorescent Y-enyne dendrimers with four and six arms)

RN 569670-23-1 CAPLUS

CN Benzene, 1,3,5-tris[4-[4-(dodecyloxy)phenyl]-2-[[4-(dodecyloxy)phenyl]ethynyl]-1-buten-3-ynyl]- (9CI) (CA INDEX NAME)

PAGE 2-A



OS.CITING REF COUNT: 16 THERE ARE 16 CAPLUS RECORDS THAT CITE THIS RECORD (16 CITINGS)  
 REFERENCE COUNT: 41 THERE ARE 41 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

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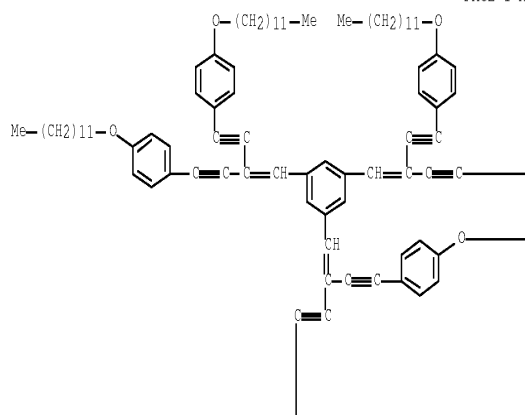
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=> file registry

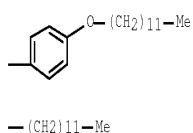
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Uploading C:\Program Files\STNEXP\Queries\10591950-claim 1-v 6.str

PAGE 1-A



PAGE 1-B



chain nodes :  
 4 5 6 7 8 9 10 11  
 chain bonds :  
 4-5 5-6 6-7 6-10 7-8 7-11 8-9  
 exact/norm bonds :  
 6-10 7-11  
 exact bonds :  
 4-5 5-6 6-7 7-8 8-9

G1:Cb,Cy,Hy

G2:C,H,O,N,Cl,Br,F,I

G3:C,H,Si,Cb,Cy,Hy



G4:H,Ak

Match level :

4:CLASS 5:CLASS 6:CLASS 7:CLASS 8:CLASS 9:CLASS 10:CLASS 11:CLASS

L1 STRUCTURE UPLOADED

=> s l1 sss full

FULL SEARCH INITIATED 15:54:41 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - 7813 TO ITERATE

100.0% PROCESSED 7813 ITERATIONS 3088 ANSWERS  
SEARCH TIME: 00.00.01

L2 3088 SEA SSS FUL L1

=> file caplus

This file contains CAS Registry Numbers for easy and accurate  
substance identification.

=> s l2

L3 814 L2

=> l3 and (electroluminescence or electroluminescent or luminescent or (light  
emitting) or OLED)

26473 ELECTROLUMINESCENCE  
30 ELECTROLUMINESCENCES  
26478 ELECTROLUMINESCENCE  
(ELECTROLUMINESCENCE OR ELECTROLUMINESCENCES)  
5 ELECTROLUMINESCENCE  
26479 ELECTROLUMINESCENCE  
(ELECTROLUMINESCENCE OR ELECTROLUMINESCENCE)  
90044 ELECTROLUMINESCENT  
8 ELECTROLUMINESCENTS  
90047 ELECTROLUMINESCENT  
(ELECTROLUMINESCENT OR ELECTROLUMINESCENTS)  
65004 LUMINESCENT  
10 LUMINESCENTS  
65010 LUMINESCENT  
(LUMINESCENT OR LUMINESCENTS)  
1334311 LIGHT  
12618 LIGHTS  
1338549 LIGHT  
(LIGHT OR LIGHTS)  
140113 EMITTING  
219 EMITTINGS  
140157 EMITTING  
(EMITTING OR EMITTINGS)  
76113 LIGHT EMITTING  
(LIGHT(W)EMITTING)  
7493 OLED  
3722 OLEDS  
9385 OLED  
(OLED OR OLEDS)

L4 3 L3 AND (ELECTROLUMINESCENCE OR ELECTROLUMINESCENT OR LUMINESCENT  
OR (LIGHT EMITTING) OR OLED)

=> d ibib abs hitstr 1-

YOU HAVE REQUESTED DATA FROM 3 ANSWERS - CONTINUE? Y/(N):y

L4 ANSWER 1 OF 3 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 2006:837081 CAPLUS Full-text

DOCUMENT NUMBER: 147:10411

TITLE: Theoretical design of light-emitting  
polymers - substitution effects of excited state  
ordering of polydiacetylene and polyacetylene

AUTHOR(S): Chen, Liping; Hou, Xinjuan; Zhu, Lingyun; Yin, Shiwei;  
Shuai, Z.

CORPORATE SOURCE: Key Laboratory of Organic Solids, Beijing National  
Laboratory for Molecular Sciences, Institute of  
Chemistry, Chinese Academy of Sciences, Beijing,  
100080, Peop. Rep. China

SOURCE: Journal of Theoretical & Computational Chemistry  
(2006), 5(Spec. Issue), 391-400  
CODEN: JTCCAC; ISSN: 0219-6336

PUBLISHER: World Scientific Publishing Co. Pte. Ltd.

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The excited states structure, essential in determining the light-emitting  
properties, in a correlated electron system behaves differently from the one-  
electron system. Previous investigations show that upon proper chemical  
substitution, the non-emissive polyacetylene (PA) can be designed to be  
strongly light-emitting materials. On the basis of the correlated quantum  
chemical calcs. within the INDO/EOM-CCSD approach, we systematically studied  
both the pristine and substituted polydiacetylene (PDA) about the low-lying  
excited states orderings. PDA possesses high mobility, but it is non-emissive.  
We predict that it is impossible to cause PDA to be light-emitting. From  
these numerical results, we propose a simple and practical rule to design  
conjugated light-emitting polymers, which require only a MO calcn. instead of  
sophisticated correlated calcs. This rule is derived from phys. pictures of  
correlated electron model, and is found to be in agreement with the existing  
expts. for various substituted PA and poly(p-phenylenebutadiynylene) (PPPB).

IT 32803-85-3, 4-Octene-2,6-diyne 337386-11-3,  
4,8-Dodecadiene-2,6,10-triye 337386-12-4,  
4,8,12-Hexadecatriene-2,6,10,14-tetrayne 337386-13-5  
337386-14-6 337386-15-7 337386-19-1  
337386-20-4 337386-21-5 337386-22-6  
337386-23-7 337386-24-8

RL: PRP (Properties)

(theor. design of light-emitting polymers -  
substitution effects of excited state ordering of polydiacetylene and  
polyacetylene)

RN 32803-85-3 CAPLUS

CN 4-Octene-2,6-diyne (CA INDEX NAME)



RN 937386-11-3 CAPLUS

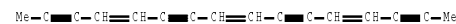
CN 4,8-Dodecadiene-2,6,10-triye (CA INDEX NAME)





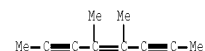
RN 937386-12-4 CAPLUS

CN 4,8,12-Hexadecatriene-2,6,10,14-tetrayne (CA INDEX NAME)



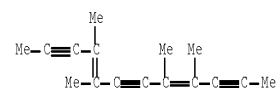
RN 937386-13-5 CAPLUS

CN 4-Octene-2,6-diyne, 4,5-dimethyl- (CA INDEX NAME)



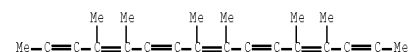
RN 937386-14-6 CAPLUS

CN 4,8-Dodecadiene-2,6,10-triyne, 4,5,8,9-tetramethyl- (CA INDEX NAME)



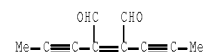
RN 937386-15-7 CAPLUS

CN 4,8,12-Hexadecatriene-2,6,10,14-tetrayne, 4,5,8,9,12,13-hexamethyl- (CA INDEX NAME)



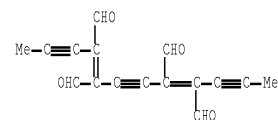
RN 937386-19-1 CAPLUS

CN 2-Butenedial, 2,3-di-1-propyn-1-yl- (CA INDEX NAME)



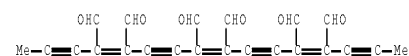
RN 937386-20-4 CAPLUS

CN 2,6-Octadien-4-ynedicarboxaldehyde, 2,7-di-1-propyn-1-yl- (CA INDEX NAME)



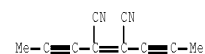
RN 937386-21-5 CAPLUS

CN 4,8,12-Hexadecatriene-2,6,10,14-tetrayne-4,5,8,9,12,13-hexacarboxaldehyde (CA INDEX NAME)



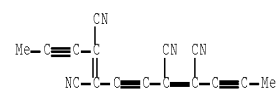
RN 937386-22-6 CAPLUS

CN 2-Butenedinitrile, 2,3-di-1-propyn-1-yl- (CA INDEX NAME)



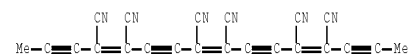
RN 937386-23-7 CAPLUS

CN 2,6-Octadien-4-ynetetraconitrile, 2,7-di-1-propyn-1-yl- (CA INDEX NAME)



RN 937386-24-8 CAPLUS

CN 4,8,12-Hexadecatriene-2,6,10,14-tetrayne-4,5,8,9,12,13-hexaconitrile (CA INDEX NAME)



OS.CITING REF COUNT: 1 THERE ARE 1 CAPLUS RECORDS THAT CITE THIS RECORD (1 CITINGS)



REFERENCE COUNT: 42 THERE ARE 42 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 2 OF 3 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 2005:1004691 CAPLUS Full-text

DOCUMENT NUMBER: 143:306181

TITLE: Process for preparation of  $\pi$ -conjugated aromatic ring-containing acetylene derivatives as organic electroluminescent devices

INVENTOR(S): Sato, Fumie; Takayama, Yuuki

PATENT ASSIGNEE(S): Nissan Chemical Industries, Ltd., Japan

SOURCE: PCT Int. Appl., 82 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

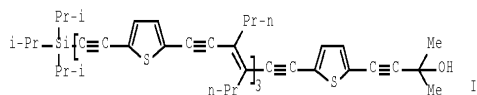
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005085176	A1	20050915	WO 2005-JP3950	20050308
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RW:	BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG			
US 20070176164	A1	20070802	US 2007-591950	20070307
PRIORITY APPLN. INFO.:			JP 2004-65446	A 20040309
			WO 2005-JP3950	W 20050308

ASSIGNMENT HISTORY FOR US PATENT AVAILABLE IN LSUS DISPLAY FORMAT

OTHER SOURCE(S): MARPAT 143:306181

GI



AB This invention pertains to a method for producing  $\pi$ -conjugated aromatic ring-containing acetylene derivs. via coupling reaction in the presence of palladium and Cu(I) catalysts. For example, the compound I was prepared in a multi-step synthesis in good yield. The title compds. are useful as electroluminescent devices.

IT	740810-64-4P	740810-65-5P	740810-67-7P
	740810-68-3P	864684-96-5P	864684-97-6P
	864684-01-5P	864684-02-6P	864684-04-8P
	864684-05-3P	864684-07-1P	864684-08-2P
	864684-31-1P	864684-32-2P	

RL: IMF (Industrial manufacture); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

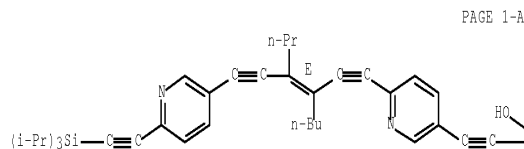
(intermediate; preparation of  $\pi$ -conjugated aromatic ring-containing acetylene

derivs. as organic electroluminescent devices)

RN 740810-64-4 CAPLUS

CN 3-Butyn-2-ol, 4-[6-[(3E)-3-butyl-4-[2-[6-[2-[tris(1-methylethyl)silyl]ethynyl]-3-pyridinyl]ethynyl]-3-hepten-1-yn-1-yl]-3-pyridinyl]-2-methyl- (CA INDEX NAME)

Double bond geometry as shown.



PAGE 1-A

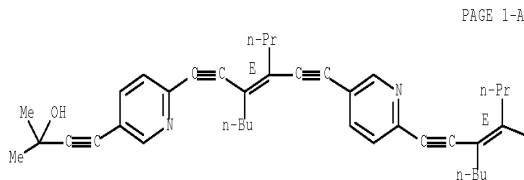
PAGE 1-B



RN 740810-65-5 CAPLUS

CN 3-Butyn-2-ol, 4-[6-[(3E)-3-butyl-4-[2-[6-[(3E)-3-butyl-4-[2-[6-[2-[tris(1-methylethyl)silyl]ethynyl]-3-pyridinyl]ethynyl]-3-hepten-1-yn-1-yl]-3-pyridinyl]ethynyl]-3-hepten-1-yn-1-yl]-3-pyridinyl]-2-methyl- (CA INDEX NAME)

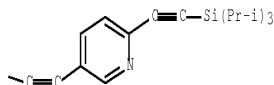
Double bond geometry as shown.



PAGE 1-A



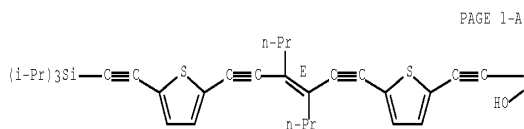
PAGE 1-B



RN 740810-67-7 CAPLUS

CN 3-Butyn-2-ol, 2-methyl-4-[5-[(3E)-3-propyl-4-[[5-[[tris(1-methylethyl)silyl]ethynyl]-2-thienyl]ethynyl]-3-hepten-1-yn-1-yl]-2-thienyl]- (CA INDEX NAME)

Double bond geometry as shown.



PAGE 1-A

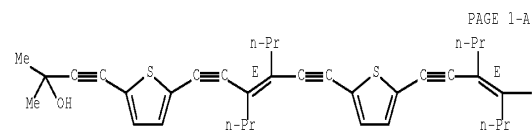


PAGE 1-B

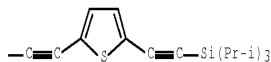
RN 740810-68-8 CAPLUS

CN 3-Butyn-2-ol, 2-methyl-4-[5-[(3E)-3-propyl-4-[[5-[(3E)-3-propyl-4-[[5-[[tris(1-methylethyl)silyl]ethynyl]-2-thienyl]ethynyl]-3-hepten-1-yn-1-yl]-2-thienyl]ethynyl]-3-hepten-1-yn-1-yl]-2-thienyl]- (CA INDEX NAME)

Double bond geometry as shown.



PAGE 1-A

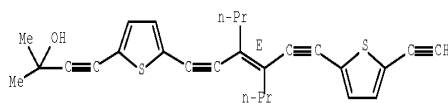


PAGE 1-B

RN 864683-96-5 CAPLUS

CN 3-Butyn-2-ol, 4-[5-[(3E)-5-ethyl-4-[2-(5-ethynyl-2-thienyl)ethynyl]-3-propyl-3-penten-1-yn-1-yl]-2-thienyl]-2-methyl- (CA INDEX NAME)

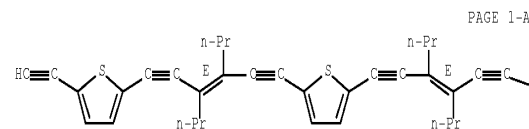
Double bond geometry as shown.



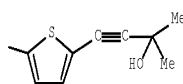
RN 864683-97-6 CAPLUS

CN 3-Butyn-2-ol, 4-[5-[(3E)-4-[2-[5-[(3E)-4-[2-(5-ethynyl-2-thienyl)ethynyl]-3-propyl-3-hepten-1-yn-1-yl]-2-thienyl]ethynyl]-3-propyl-3-hepten-1-yn-1-yl]-2-thienyl]-2-methyl- (CA INDEX NAME)

Double bond geometry as shown.



PAGE 1-A

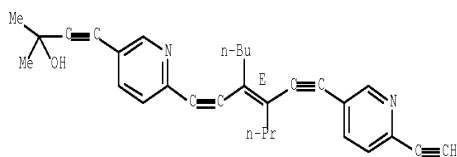


PAGE 1-B

RN 864684-01-5 CAPLUS

CN 3-Butyn-2-ol, 4-[6-[(3E)-3-butyl-4-[2-(6-ethynyl-3-pyridinyl)ethynyl]-3-hepten-1-yn-1-yl]-3-pyridinyl]-2-methyl- (CA INDEX NAME)

Double bond geometry as shown.

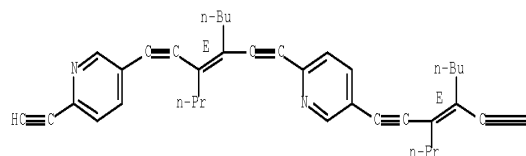




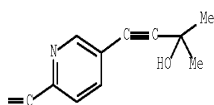
RN 864684-02-6 CAPLUS  
 CN 3-Butyn-2-ol, 4-[6-[(3E)-3-butyl-4-[2-[6-[(3E)-3-butyl-4-[2-(6-ethynyl-3-pyridinyl)ethynyl]-3-hepten-1-yn-1-yl]-3-pyridinyl]ethynyl]-3-hepten-1-yn-1-yl]-3-pyridinyl]-2-methyl- (CA INDEX NAME)

Double bond geometry as shown.

PAGE 1-A

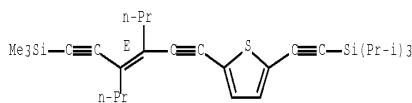


PAGE 1-B



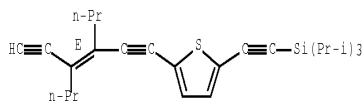
RN 864684-04-8 CAPLUS  
 CN Thiophene, 2-[(3E)-3,4-dipropyl-6-(trimethylsilyl)-3-hexene-1,5-diyn-1-yl]-5-[2-[tris(1-methylethyl)silyl]ethynyl]- (CA INDEX NAME)

Double bond geometry as shown.



RN 864684-05-9 CAPLUS  
 CN Thiophene, 2-[(3E)-4-ethynyl-3-propyl-3-hepten-1-yn-1-yl]-5-[2-[tris(1-methylethyl)silyl]ethynyl]- (CA INDEX NAME)

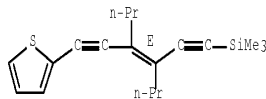
Double bond geometry as shown.



RN 864684-07-1 CAPLUS

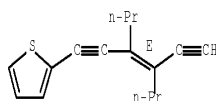
CN Thiophene, 2-[(3E)-5-ethyl-3-propyl-4-[2-(trimethylsilyl)ethynyl]-3-penten-1-yn-1-yl]- (CA INDEX NAME)

Double bond geometry as shown.



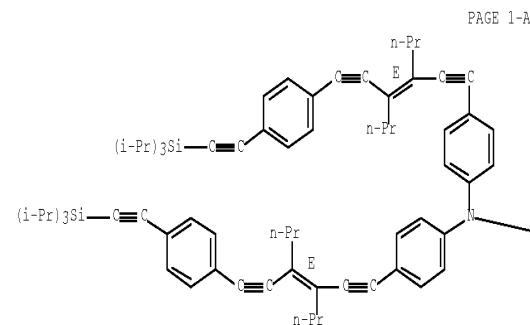
RN 864684-08-2 CAPLUS  
 CN Thiophene, 2-[(3E)-4-ethynyl-3-propyl-3-hepten-1-yn-1-yl]- (CA INDEX NAME)

Double bond geometry as shown.



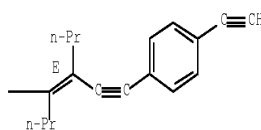
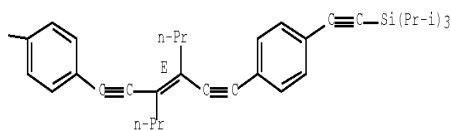
RN 864684-31-1 CAPLUS  
 CN Benzenamine, N-[4-[(3E)-3,4-dipropyl-6-[4-[2-[tris(1-methylethyl)silyl]ethynyl]phenyl]-3-hexene-1,5-diyn-1-yl]phenyl]-4-[(3E)-3-propyl-4-[2-[4-[2-[tris(1-methylethyl)silyl]ethynyl]phenyl]ethynyl]-3-hepten-1-yn-1-yl]-N-[4-[(3E)-3-propyl-4-[2-[4-[2-[tris(1-methylethyl)silyl]ethynyl]phenyl]ethynyl]-3-hepten-1-yn-1-yl]phenyl]- (CA INDEX NAME)

Double bond geometry as shown.



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RN 864684-32-2 CAPLUS

CN Benzenamine, N-[4-[(3E)-5-ethyl-4-[2-(4-ethynylphenyl)ethynyl]-3-propyl-3-penten-1-yn-1-yl]phenyl]-4-[(3E)-4-[2-(4-ethynylphenyl)ethynyl]-3-propyl-3-hepten-1-yn-1-yl]-N-[4-[(3E)-4-[2-(4-ethynylphenyl)ethynyl]-3-propyl-3-hepten-1-yn-1-yl]phenyl]- (CA INDEX NAME)

Double bond geometry as shown.

IT 740810-66-6F 740610-69-9F 864684-03-7P  
864684-06-0F 864684-03-3F 864684-01-9P  
864684-22-0F 864684-23-1P 864684-04-0P  
864684-25-3P 864684-26-4P 864684-27-5F  
864684-28-6P 864684-29-7P 864684-30-0P  
864684-33-3P

RL: DEV (Device component use); IMF (Industrial manufacture); SPN (Synthetic preparation); TEM (Technical or engineered material use); PREP (Preparation); USES (Uses)

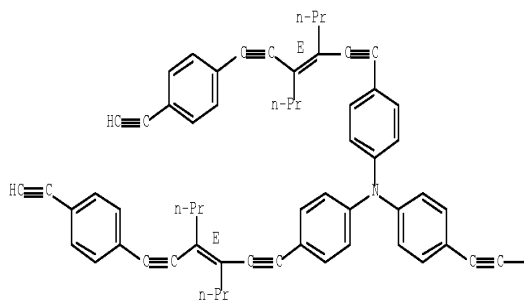
(preparation of  $\pi$ -conjugated aromatic ring-containing acetylene derivs. as organic electroluminescent devices)

RN 740810-66-6 CAPLUS

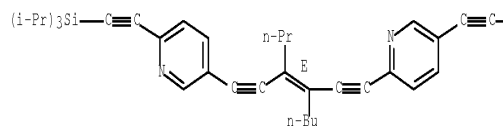
CN 3-Butyn-2-ol, 4-[6-[(3E)-3-butyl-4-[2-[6-[(3E)-3-butyl-4-[2-[6-[(3E)-3-butyl-4-[2-[6-[2-[tris(1-methylethyl)silyl]ethynyl]-3-pyridinyl]ethynyl]-3-hepten-1-yn-1-yl]-3-pyridinyl]ethynyl]-3-hepten-1-yn-1-yl]-3-pyridinyl]ethynyl]-3-hepten-1-yn-1-yl]-3-pyridinyl]-2-methyl- (CA INDEX NAME)

Double bond geometry as shown.

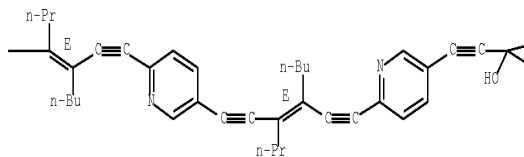
PAGE 1-A



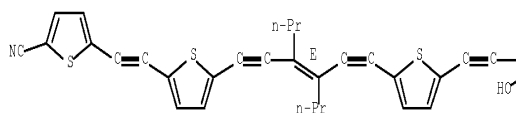
PAGE 1-A



PAGE 1-B



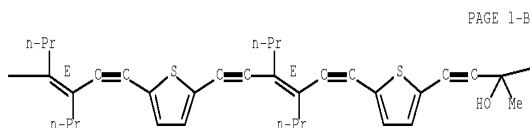
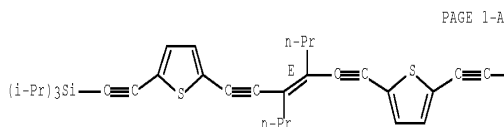




RN 740810-69-9 CAPLUS

CN 3-Butyn-2-ol, 4-[5-[(3E)-4-[2-[5-[(3E)-5-ethyl-4-[2-[5-[(3E)-5-ethyl-3-propyl-4-[2-[5-[2-[tris(1-methylethyl)silyl]ethynyl]-2-thienyl]ethynyl]-3-penten-1-yn-1-yl]-2-thienyl]ethynyl]-3-propyl-3-penten-1-yn-1-yl]-2-thienyl]ethynyl]-3-propyl-3-hepten-1-yn-1-yl]-2-thienyl]-2-methyl- (CA INDEX NAME)

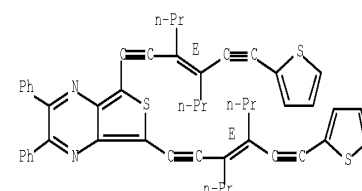
Double bond geometry as shown.



RN 864684-03-7 CAPLUS

CN 2-Thiophenecarbonitrile, 5-[2-[5-[(3E)-5-ethyl-4-[2-[5-(3-hydroxy-3-methyl-1-butyn-1-yl)-2-thienyl]ethynyl]-3-propyl-3-penten-1-yn-1-yl]-2-thienyl]ethynyl]- (CA INDEX NAME)

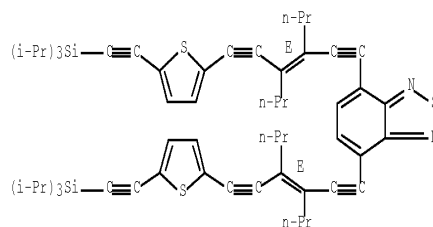
Double bond geometry as shown.



RN 864684-06-0 CAPLUS

CN 2,1,3-Benzothiadiazole, 4-[(3E)-3,4-dipropyl-6-[5-[2-[tris(1-methylethyl)silyl]ethynyl]-2-thienyl]-3-hexene-1,5-diyn-1-yl]-7-[(3E)-3-propyl-4-[2-[5-[2-[tris(1-methylethyl)silyl]ethynyl]-2-thienyl]ethynyl]-3-hepten-1-yn-1-yl]- (CA INDEX NAME)

Double bond geometry as shown.



RN 864684-09-3 CAPLUS

CN Thieno[3,4-b]pyrazine, 5-[(3E)-3,4-dipropyl-6-(2-thienyl)-3-hexene-1,5-diyn-1-yl]-2,3-diphenyl-7-[(3E)-3-propyl-4-[2-(2-thienyl)ethynyl]-3-hepten-1-yn-1-yl]- (CA INDEX NAME)

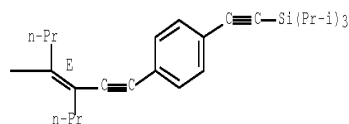
Double bond geometry as shown.



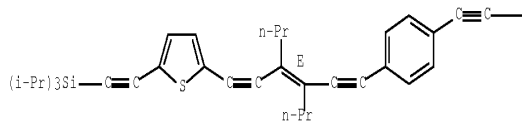
RN 864684-21-9 CAPLUS

CN Thiophene, 2-[(3E)-3,4-dipropyl-6-[4-[(3E)-3-propyl-4-[2-[5-[2-[tris(1-methylethyl)silyl]ethynyl]-2-thienyl]ethynyl]-3-hepten-1-yn-1-yl]phenyl]-3-hexene-1,5-diyn-1-yl]-5-[2-[tris(1-methylethyl)silyl]ethynyl]- (CA INDEX NAME)

Double bond geometry as shown.



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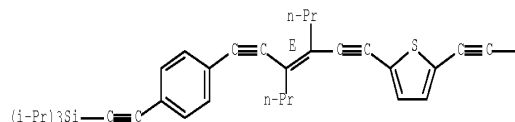


RN 864684-23-1 CAPLUS

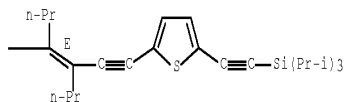
CN Thiophene, 2-[(3E)-3,4-dipropyl-6-[4-[2-[tris(1-methylethyl)silyl]ethynyl]phenyl]-3-hexene-1,5-diyn-1-yl]-5-[(3E)-3-propyl-4-[2-[4-[2-[tris(1-methylethyl)silyl]ethynyl]phenyl]ethynyl]-3-hepten-1-yn-1-yl]- (CA INDEX NAME)

Double bond geometry as shown.

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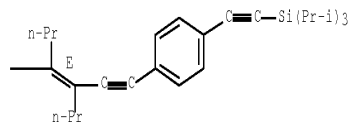


RN 864684-22-0 CAPLUS

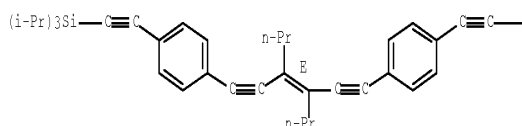
CN Benzene, 1-[(3E)-3,4-dipropyl-6-[4-[2-[tris(1-methylethyl)silyl]ethynyl]phenyl]-3-hexene-1,5-diyn-1-yl]-4-[(3E)-3-propyl-4-[2-[4-[2-[tris(1-methylethyl)silyl]ethynyl]phenyl]ethynyl]-3-hepten-1-yn-1-yl]- (CA INDEX NAME)

Double bond geometry as shown.

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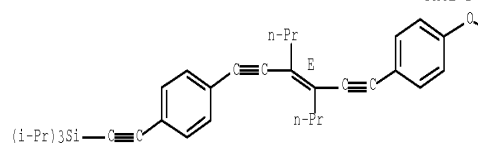


RN 864684-24-2 CAPLUS

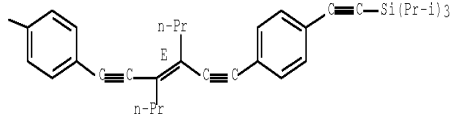
CN Silane, [oxybis[4,1-phenylene[(3E)-3,4-dipropyl-3-hexene-1,5-diyne-6,1-diyl]-4,1-phenylene-2,1-ethynediyl]]bis[tris(1-methylethyl)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

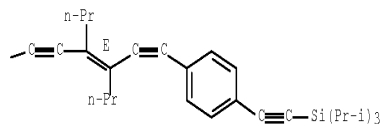
PAGE 1-A







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PAGE 1-B

RN 864684-25-3 CAPLUS

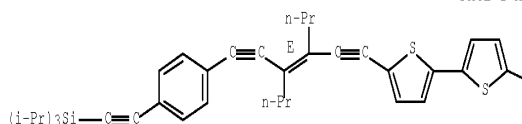
CN 2,2'-Bithiophene, 5-[(3E)-3,4-dipropyl-6-[4-[2-[tris(1-methylethyl)silyl]ethynyl]phenyl]-3-hexene-1,5-diyn-1-yl]-5'-[(3E)-3-propyl-4-[2-[4-[2-[tris(1-methylethyl)silyl]ethynyl]phenyl]ethynyl]-3-hepten-1-yn-1-yl]- (CA INDEX NAME)

Double bond geometry as shown.

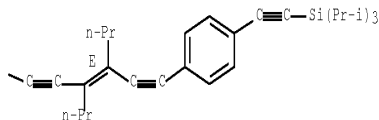
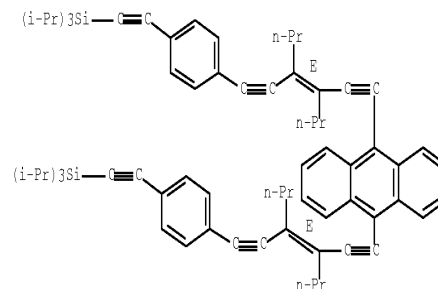
RN 864684-27-5 CAPLUS

CN Anthracene, 9-[(3E)-3,4-dipropyl-6-[4-[2-[tris(1-methylethyl)silyl]ethynyl]phenyl]-3-hexene-1,5-diyn-1-yl]-10-[(3E)-3-propyl-4-[2-[4-[2-[tris(1-methylethyl)silyl]ethynyl]phenyl]ethynyl]-3-hepten-1-yn-1-yl]- (CA INDEX NAME)

Double bond geometry as shown.



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RN 864684-26-4 CAPLUS

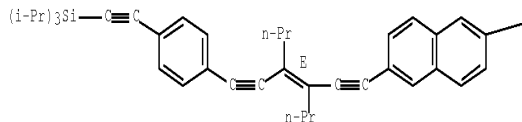
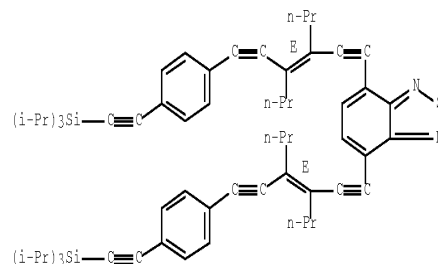
CN Naphthalene, 2-[(3E)-3,4-dipropyl-6-[4-[2-[tris(1-methylethyl)silyl]ethynyl]phenyl]-3-hexene-1,5-diyn-1-yl]-6-[(3E)-3-propyl-4-[2-[4-[2-[tris(1-methylethyl)silyl]ethynyl]phenyl]ethynyl]-3-hepten-1-yn-1-yl]- (CA INDEX NAME)

Double bond geometry as shown.

RN 864684-28-6 CAPLUS

CN 2,1,3-Benzothiadiazole, 4-[(3E)-3,4-dipropyl-6-[4-[2-[tris(1-methylethyl)silyl]ethynyl]phenyl]-3-hexene-1,5-diyn-1-yl]-7-[(3E)-3-propyl-4-[2-[4-[2-[tris(1-methylethyl)silyl]ethynyl]phenyl]ethynyl]-3-hepten-1-yn-1-yl]- (CA INDEX NAME)

Double bond geometry as shown.



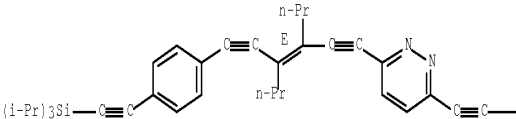
PAGE 1-A

RN 864684-29-7 CAPLUS

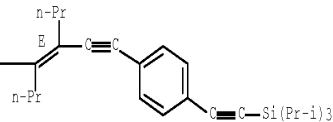


CN Pyridazine, 3-[(3E)-3,4-dipropyl-6-[4-[2-[tris(1-methylethyl)silyl]ethynyl]phenyl]-3-hexene-1,5-diyn-1-yl]-6-[(3E)-3-propyl-4-[2-[4-[2-[tris(1-methylethyl)silyl]ethynyl]phenyl]ethynyl]-3-hepten-1-yn-1-yl]- (CA INDEX NAME)

Double bond geometry as shown.

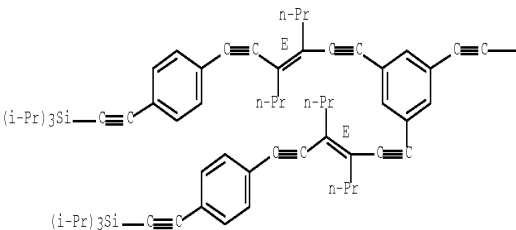


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RN 864684-30-0 CAPLUS  
CN Benzene, 1-[(3E)-3,4-dipropyl-6-[4-[2-[tris(1-methylethyl)silyl]ethynyl]phenyl]-3-hexene-1,5-diyn-1-yl]-3-[(3E)-5-ethyl-3-propyl-4-[2-[4-[2-[tris(1-methylethyl)silyl]ethynyl]phenyl]ethynyl]-3-penten-1-yn-1-yl]-5-[(3E)-3-propyl-4-[2-[4-[2-[tris(1-methylethyl)silyl]ethynyl]phenyl]ethynyl]-3-hepten-1-yn-1-yl]- (CA INDEX NAME)

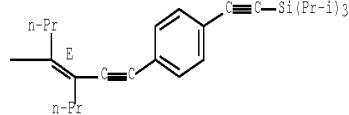
Double bond geometry as shown.



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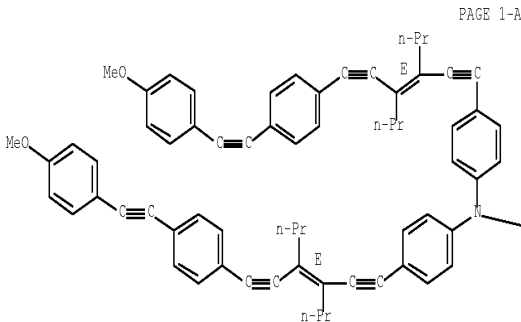
PAGE 1-B



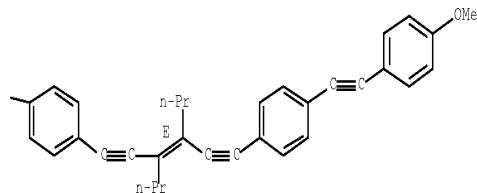
PAGE 1-B

RN 864684-33-3 CAPLUS  
CN Benzenamine, N-[4-[(3E)-5-ethyl-4-[2-[4-[2-(4-methoxyphenyl)ethynyl]phenyl]ethynyl]-3-propyl-3-penten-1-yn-1-yl]phenyl]-4-[(3E)-4-[2-[4-[2-(4-methoxyphenyl)ethynyl]phenyl]ethynyl]-3-propyl-3-hepten-1-yn-1-yl]-N-[4-[(3E)-4-[2-[4-[2-(4-methoxyphenyl)ethynyl]phenyl]ethynyl]-3-propyl-3-hepten-1-yn-1-yl]phenyl]- (CA INDEX NAME)

Double bond geometry as shown.



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PAGE 2-A

ACCESSION NUMBER: 2003:189466 CAPLUS Full-text

DOCUMENT NUMBER: 139:101213

TITLE: Luminescent properties of carbon-rich starburst gold(I) acetylide complexes. Crystal structure of [TEE][Au(PCy3)]4 ([TEE]H4 = tetraethynylethene)

AUTHOR(S): Lu, Wei; Zhu, Nianyong; Che, Chi-Ming

CORPORATE SOURCE: Department of Chemistry and HKU-CAS Joint Laboratory on New Materials, The University of Hong Kong, Hong Kong, Peop. Rep. China

SOURCE: Journal of Organometallic Chemistry (2003), 670(1-2), 11-16

CODEN: JORCAI; ISSN: 0022-328X

PUBLISHER: Elsevier Science B.V.

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 139:101213

AB Two carbon-rich starburst gold(I) acetylide complexes [TEE][Au(PCy3)]4 (3, [TEE]H4 = tetraethynylethene) and [TEB][Au(PCy3)]3 (6, [TEB]H3 = 1,3,5-triethynylbenzene) were prepared and their UV-vis absorption, emission and excitation spectra have been recorded. In fluid CH2Cl2 solns., 3 exhibits prompt 1( $\pi\pi^*$ ) fluorescence with  $\lambda_0-0$  and  $\lambda_{max}$  at 413 and 428 nm, resp., while 6 displays 3( $\pi\pi^*$ ) phosphorescence with  $\lambda_0-0$  and  $\lambda_{max}$  at 446 and 479 nm, resp. The crystal structure of 3-CH2Cl2 has been determined

IT 558460-17-6P

RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)  
(crystal structure; preparation and luminescent properties of carbon-rich starburst gold acetylide complexes and crystal structure of tetraethynylethene gold phosphine complex)

RN 558460-17-6 CAPLUS

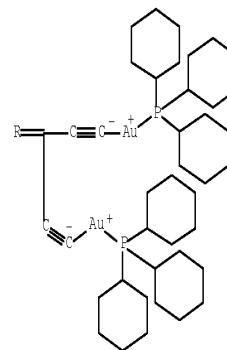
CN Gold, [ $\mu$ -[3,4-di(ethynyl- $\kappa$ C2)-3-hexene-1,5-diynato(4-)- $\kappa$ C1, $\kappa$ C6]]tetrakis(tricyclohexylphosphine)tetra-, compd. with dichloromethane (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 558460-16-5

CMF C82 H132 Au4 P4

CCI CCS



CM 2

CRN 75-09-2

CMF C H2 Cl2

Cl-CH2-Cl

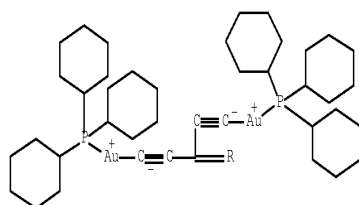
IT 558460-16-5P

RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)  
(mol. structure, luminescence; preparation and luminescent properties of carbon-rich starburst gold acetylide complexes and crystal structure of tetraethynylethene gold phosphine complex)

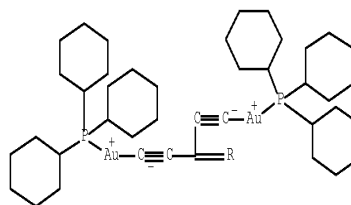
RN 558460-16-5 CAPLUS

CN Gold, [ $\mu$ -[3,4-di(ethynyl- $\kappa$ C2)-3-hexene-1,5-diynato(4-)- $\kappa$ C1, $\kappa$ C6]]tetrakis(tricyclohexylphosphine)tetra- (9CI) (CA INDEX NAME)

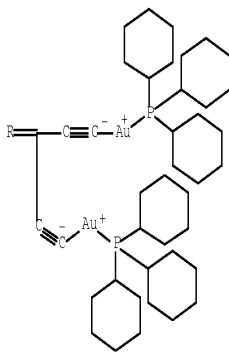
PAGE 1-A



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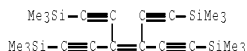
IT 55660-76-9

RL: RCT (Reactant); RACT (Reactant or reagent)

(preparation and luminescent properties of carbon-rich starburst  
gold acetylide complexes and crystal structure of tetraethynylethane  
gold phosphine complex)

RN 55660-76-9 CAPLUS

CN Silane, 1,1'-[3,4-bis[2-(trimethylsilyl)ethynyl]-3-hexene-2,5-diyne-1,6-  
diyl]bis[1,1,1-trimethyl- (CA INDEX NAME)



OS.CITING REF COUNT: 30 THERE ARE 30 CAPLUS RECORDS THAT CITE THIS  
RECORD (30 CITINGS)  
REFERENCE COUNT: 34 THERE ARE 34 CITED REFERENCES AVAILABLE FOR THIS  
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> 13 and (electroluminescence or electroluminescent or luminescent or (light  
emitting) or OLED or (non linear optics) or NLO)

26473 ELECTROLUMINESCENCE  
30 ELECTROLUMINESCENCES  
26478 ELECTROLUMINESCENCE  
(ELECTROLUMINESCENCE OR ELECTROLUMINESCENCES)  
5 ELECTROLUMINESCENCE  
26479 ELECTROLUMINESCENCE  
(ELECTROLUMINESCENCE OR ELECTROLUMINESCENCE)  
90044 ELECTROLUMINESCENT  
8 ELECTROLUMINESCENTS  
90047 ELECTROLUMINESCENT  
(ELECTROLUMINESCENT OR ELECTROLUMINESCENTS)  
65004 LUMINESCENT  
10 LUMINESCENTS  
65010 LUMINESCENT  
(LUMINESCENT OR LUMINESCENTS)

1334311 LIGHT  
12618 LIGHTS  
1338549 LIGHT  
(LIGHT OR LIGHTS)  
140113 EMITTING  
219 EMISSIONS  
140157 EMITTING  
(EMITTING OR EMISSIONS)  
76113 LIGHT EMITTING  
(LIGHT(W)EMITTING)  
7493 OLED  
3722 OLEDS  
9385 OLED  
(OLED OR OLEDS)  
1110208 NON  
38 NONS  
1110237 NON  
(NON OR NONS)

710357 LINEAR  
74 LINEARS  
710397 LINEAR  
(LINEAR OR LINEARS)  
53122 OPTICS  
311 NON LINEAR OPTICS  
(NON(W)LINEAR(W)OPTICS)  
7807 NLO  
19 NLOS  
7820 NLO  
(NLO OR NLOS)

L5 6 L3 AND (ELECTROLUMINESCENCE OR ELECTROLUMINESCENT OR LUMINESCENT  
OR (LIGHT EMITTING) OR OLED OR (NON LINEAR OPTICS) OR NLO)

=&gt; d ibib abs hitstr 1-

YOU HAVE REQUESTED DATA FROM 6 ANSWERS - CONTINUE? Y/(N):y

L5 ANSWER 1 OF 6 CAPLUS COPYRIGHT 2009 ACS on STN  
ACCESSION NUMBER: 2006:837081 CAPLUS Full-text  
DOCUMENT NUMBER: 147:10411  
TITLE: Theoretical design of light-emitting  
polymers - substitution effects of excited state  
ordering of polydiacetylene and polyacetylene  
AUTHOR(S): Chen, Liping; Hou, Xinjuan; Zhu, Lingyun; Yin, Shiwei;  
Shuai, Z.  
CORPORATE SOURCE: Key Laboratory of Organic Solids, Beijing National  
Laboratory for Molecular Sciences, Institute of  
Chemistry, Chinese Academy of Sciences, Beijing,  
100080, Peop. Rep. China  
SOURCE: Journal of Theoretical & Computational Chemistry  
(2006), 5(Spec. Issue), 391-400  
CODEN: JTCCAC; ISSN: 0219-6336  
PUBLISHER: World Scientific Publishing Co. Pte. Ltd.  
DOCUMENT TYPE: Journal  
LANGUAGE: English  
AB The excited states structure, essential in determining the light-emitting  
properties, in a correlated electron system behaves differently from the one-  
electron system. Previous investigations show that upon proper chemical  
substitution, the non-emissive polyacetylene (PA) can be designed to be  
strongly light-emitting materials. On the basis of the correlated quantum  
chemical calcs. within the INDO/EOM-CCSD approach, we systematically studied  
both the pristine and substituted polydiacetylene (PDA) about the low-lying



excited states orderings. PDA possesses high mobility, but it is non-emissive. We predict that it is impossible to cause PDA to be light-emitting. From these numerical results, we propose a simple and practical rule to design conjugated light-emitting polymers, which require only a MO calcn. instead of sophisticated correlated calcns. This rule is derived from phys. pictures of correlated electron model, and is found to be in agreement with the existing expts. for various substituted PA and poly(p-phenylenebutadiynylene) (PPPB).

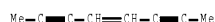
IT 33803-85-3, 4-Octene-2,6-diyne 937386-11-3,  
4,8-Dodecadiene-2,6,10-triyne 937386-12-4,  
4,8,12-Hexadecatriene-2,6,10,14-tetrayne 937386-13-5  
937386-14-6 937386-15-7 937386-16-1  
937386-20-4 937386-21-5 937386-22-6  
937386-23-7 937386-24-8

RL: PRP (Properties)

(theor. design of light-emitting polymers -  
substitution effects of excited state ordering of polydiacetylene and  
polyacetylene)

RN 32803-85-3 CAPLUS

CN 4-Octene-2,6-diyne (CA INDEX NAME)



RN 937386-11-3 CAPLUS

CN 4,8-Dodecadiene-2,6,10-triyne (CA INDEX NAME)



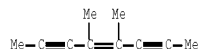
RN 937386-12-4 CAPLUS

CN 4,8,12-Hexadecatriene-2,6,10,14-tetrayne (CA INDEX NAME)



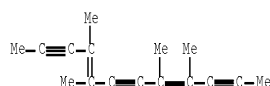
RN 937386-13-5 CAPLUS

CN 4-Octene-2,6-diyne, 4,5-dimethyl- (CA INDEX NAME)



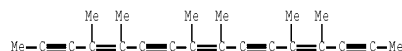
RN 937386-14-6 CAPLUS

CN 4,8-Dodecadiene-2,6,10-triyne, 4,5,8,9-tetramethyl- (CA INDEX NAME)



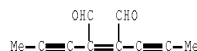
RN 937386-15-7 CAPLUS

CN 4,8,12-Hexadecatriene-2,6,10,14-tetrayne, 4,5,8,9,12,13-hexamethyl- (CA INDEX NAME)



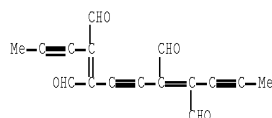
RN 937386-19-1 CAPLUS

CN 2-Butenedial, 2,3-di-1-propyn-1-yl- (CA INDEX NAME)



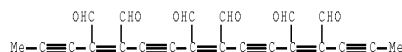
RN 937386-20-4 CAPLUS

CN 2,6-Octadien-4-ynedicarboxaldehyde, 2,7-di-1-propyn-1-yl- (CA INDEX NAME)



RN 937386-21-5 CAPLUS

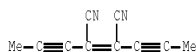
CN 4,8,12-Hexadecatriene-2,6,10,14-tetrayne-4,5,8,9,12,13-hexacarboxaldehyde (CA INDEX NAME)



RN 937386-22-6 CAPLUS

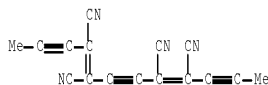
CN 2-Butenedinitrile, 2,3-di-1-propyn-1-yl- (CA INDEX NAME)





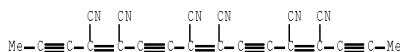
RN 937386-23-7 CAPLUS

CN 2,6-Octadien-4-ynetetra-carbonitrile, 2,7-di-1-propyn-1-yl- (CA INDEX NAME)



RN 937386-24-8 CAPLUS

CN 4,8,12-Hexadecatriene-2,6,10,14-tetrayne-4,5,8,9,12,13-hexa-carbonitrile (CA INDEX NAME)



OS.CITING REF COUNT: 1 THERE ARE 1 CAPLUS RECORDS THAT CITE THIS RECORD (1 CITINGS)

REFERENCE COUNT: 42 THERE ARE 42 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 2 OF 6 CAPLUS COPYRIGHT 2009 ACS ON STN

ACCESSION NUMBER: 2005:1004691 CAPLUS [Full-text](#)

DOCUMENT NUMBER: 143:306181

TITLE: Process for preparation of  $\pi$ -conjugated aromatic ring-containing acetylene derivatives as organic electroluminescent devices

INVENTOR(S): Sato, Fumie; Takayama, Yuuki

PATENT ASSIGNEE(S): Nissan Chemical Industries, Ltd., Japan

SOURCE: PCT Int. Appl., 82 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005085176	A1	20050915	WO 2005-JP3950	20050308
W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW			

RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, L7, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

US 20070176164 A1 20070802 US 2007-591950 20070307

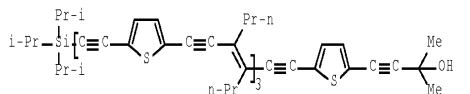
PRIORITY APPLN. INFO.: JP 2004-65446 A 20040309

WO 2005-JP3950 W 20050308

ASSIGNMENT HISTORY FOR US PATENT AVAILABLE IN LSUS DISPLAY FORMAT

OTHER SOURCE(S): MARPAT 143:306181

GI



AB This invention pertains to a method for producing  $\pi$ -conjugated aromatic ring-containing acetylene derivs. via coupling reaction in the presence of palladium and Cu(I) catalysts. For example, the compound I was prepared in a multi-step synthesis in good yield. The title compds. are useful as electroluminescent devices.

IT 740810-64-4P 740317-65-5P 740810-67-7P

740810-68-8P 864683-96-5P 864683-97-6P

864684-01-8P 864684-02-6P 864684-04-8P

864684-05-9P 864684-07-1P 864684-03-2P

864684-31-1P 864684-32-2P

RL: IMF (Industrial manufacture); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(intermediate; preparation of  $\pi$ -conjugated aromatic ring-containing acetylene

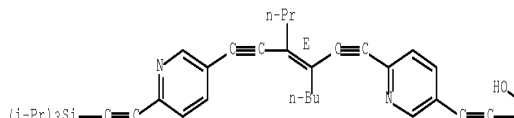
derivs. as organic electroluminescent devices)

RN 740810-64-4 CAPLUS

CN 3-Butyn-2-ol, 4-[6-[(3E)-3-butyl-4-[2-[6-[2-[tris(1-methylethyl)silyl]ethynyl]-3-pyridinyl]ethynyl]-3-hepten-1-yn-1-yl]-3-pyridinyl]-2-methyl- (CA INDEX NAME)

Double bond geometry as shown.

PAGE 1-A



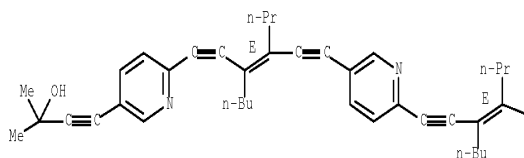




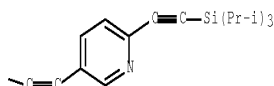
RN 740810-65-5 CAPLUS

CN 3-Butyn-2-ol, 4-[6-[(3E)-3-butyl-4-[2-[6-[(3E)-3-butyl-4-[2-[6-[2-[tris(1-methylethyl)silyl]ethynyl]-3-pyridinyl]ethynyl]-3-hepten-1-yn-1-yl]-3-pyridinyl]ethynyl]-3-hepten-1-yn-1-yl]-3-pyridinyl]-2-methyl- (CA INDEX NAME)

Double bond geometry as shown.



PAGE 1-A

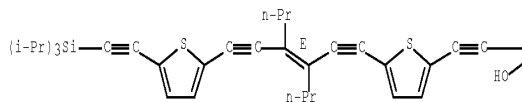


PAGE 1-B

RN 740810-67-7 CAPLUS

CN 3-Butyn-2-ol, 2-methyl-4-[5-[(3E)-3-propyl-4-[[5-[[tris(1-methylethyl)silyl]ethynyl]-2-thienyl]ethynyl]-3-hepten-1-yn-1-yl]-2-thienyl]- (CA INDEX NAME)

Double bond geometry as shown.



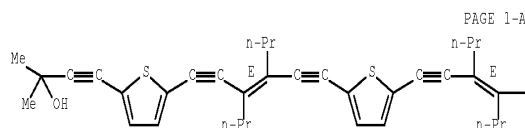
PAGE 1-A



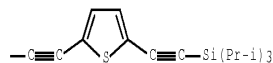
RN 740810-68-8 CAPLUS

CN 3-Butyn-2-ol, 2-methyl-4-[5-[(3E)-3-propyl-4-[[5-[(3E)-3-propyl-4-[[5-[[tris(1-methylethyl)silyl]ethynyl]-2-thienyl]ethynyl]-3-hepten-1-yn-1-yl]-2-thienyl]ethynyl]-3-hepten-1-yn-1-yl]-2-thienyl]- (CA INDEX NAME)

Double bond geometry as shown.



PAGE 1-A

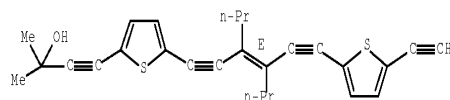


PAGE 1-B

RN 864683-96-5 CAPLUS

CN 3-Butyn-2-ol, 4-[5-[(3E)-5-ethyl-4-[2-(5-ethynyl-2-thienyl)ethynyl]-3-propyl-3-penten-1-yn-1-yl]-2-thienyl]-2-methyl- (CA INDEX NAME)

Double bond geometry as shown.

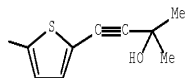
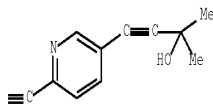
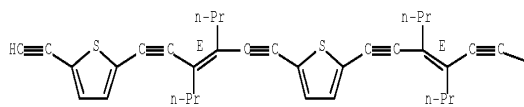


RN 864683-97-6 CAPLUS

CN 3-Butyn-2-ol, 4-[5-[(3E)-4-[2-[5-[(3E)-4-[2-(5-ethynyl-2-thienyl)ethynyl]-3-propyl-3-hepten-1-yn-1-yl]-2-thienyl]ethynyl]-3-propyl-3-hepten-1-yn-1-yl]-2-thienyl]-2-methyl- (CA INDEX NAME)

Double bond geometry as shown.

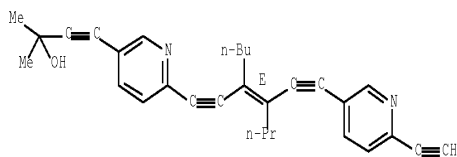




RN 864684-01-5 CAPLUS

CN 3-Butyn-2-ol, 4-[6-[(3E)-3-butyl-4-[2-(6-ethynyl-3-pyridinyl)ethynyl]-3-hepten-1-yn-1-yl]-3-pyridinyl]-2-methyl- (CA INDEX NAME)

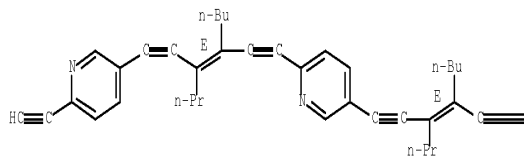
Double bond geometry as shown.



RN 864684-02-6 CAPLUS

CN 3-Butyn-2-ol, 4-[6-[(3E)-3-butyl-4-[2-[6-[(3E)-3-butyl-4-[2-(6-ethynyl-3-pyridinyl)ethynyl]-3-hepten-1-yn-1-yl]-3-pyridinyl]ethynyl]-3-hepten-1-yn-1-yl]-3-pyridinyl]-2-methyl- (CA INDEX NAME)

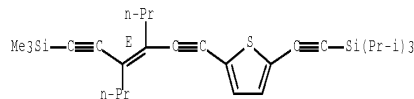
Double bond geometry as shown.



RN 864684-04-8 CAPLUS

CN Thiophene, 2-[(3E)-3,4-dipropyl-6-(trimethylsilyl)-3-hexene-1,5-diyn-1-yl]-5-[2-[tris(1-methylethyl)silyl]ethynyl]- (CA INDEX NAME)

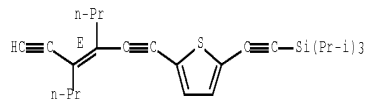
Double bond geometry as shown.



RN 864684-05-9 CAPLUS

CN Thiophene, 2-[(3E)-4-ethynyl-3-propyl-3-hepten-1-yn-1-yl]-5-[2-[tris(1-methylethyl)silyl]ethynyl]- (CA INDEX NAME)

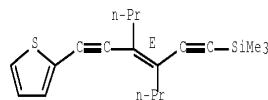
Double bond geometry as shown.



RN 864684-07-1 CAPLUS

CN Thiophene, 2-[(3E)-5-ethyl-3-propyl-4-[2-(trimethylsilyl)ethynyl]-3-penten-1-yn-1-yl]- (CA INDEX NAME)

Double bond geometry as shown.

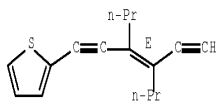


RN 864684-08-2 CAPLUS

CN Thiophene, 2-[(3E)-4-ethynyl-3-propyl-3-hepten-1-yn-1-yl]- (CA INDEX NAME)

Double bond geometry as shown.





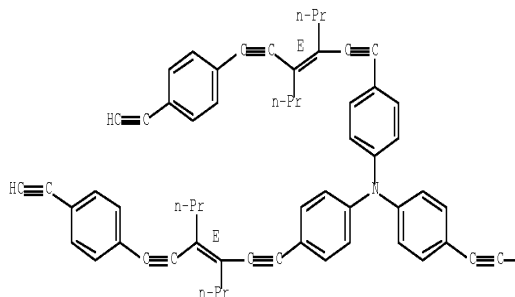
hepten-1-yn-1-yl]-N-[4-[(3E)-4-[2-(4-ethynylphenyl)ethynyl]-3-propyl-3-hepten-1-yn-1-yl]phenyl]- (CA INDEX NAME)

Double bond geometry as shown.

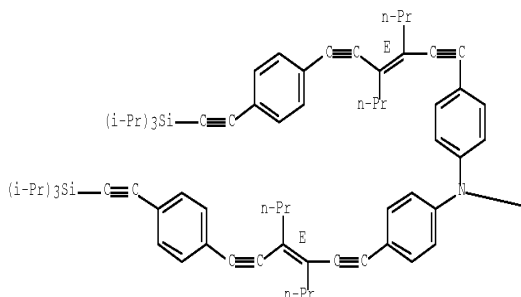
PAGE 1-A

RN 864684-31-1 CAPLUS  
CN Benzenamine, N-[4-[(3E)-3,4-dipropyl-6-[4-[2-[tris(1-methylethyl)silyl]ethynyl]phenyl]-3-hexene-1,5-diyn-1-yl]phenyl]-4-[(3E)-3-propyl-4-[2-[4-[2-[tris(1-methylethyl)silyl]ethynyl]phenyl]ethynyl]-3-hepten-1-yn-1-yl]-N-[4-[(3E)-3-propyl-4-[2-[4-[2-[tris(1-methylethyl)silyl]ethynyl]phenyl]ethynyl]-3-hepten-1-yn-1-yl]phenyl]- (CA INDEX NAME)

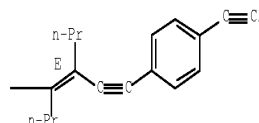
Double bond geometry as shown.



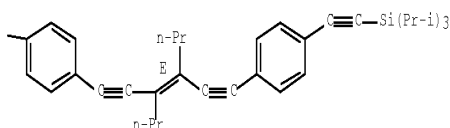
PAGE 1-A



PAGE 1-B



PAGE 1-B



IT 740810-66-6P 740810-63-3P 864684-03-7P  
864684-06-0P 864684-09-3P 864684-21-9P  
864684-22-0P 864684-23-1P 864684-24-2P  
864684-25-3P 864684-26-4P 864684-27-5P  
864684-28-6P 864684-29-7P 864684-30-0P  
864684-33-3P

RL: DEV (Device component use); IMF (Industrial manufacture); SPN (Synthetic preparation); TEM (Technical or engineered material use); PREP (Preparation); USES (Uses)

(preparation of  $\pi$ -conjugated aromatic ring-containing acetylene derivs. as organic electroluminescent devices)

RN 740810-66-6 CAPLUS

RN 864684-32-2 CAPLUS  
CN Benzenamine, N-[4-[(3E)-5-ethyl-4-[2-(4-ethynylphenyl)ethynyl]-3-propyl-3-penten-1-yn-1-yl]phenyl]-4-[(3E)-4-[2-(4-ethynylphenyl)ethynyl]-3-propyl-3-

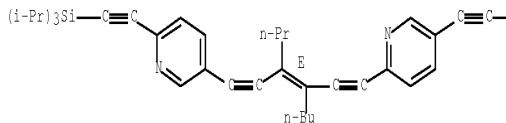
3-Butyn-2-ol, 4-[6-[(3E)-3-butyl-4-[2-[6-[(3E)-3-butyl-4-[2-[6-[(3E)-3-butyl-4-[2-[6-[2-[tris(1-methylethyl)silyl]ethynyl]-3-pyridinyl]ethynyl]-3-hepten-1-yn-1-yl]-3-pyridinyl]ethynyl]-3-hepten-1-yn-1-yl]-3-



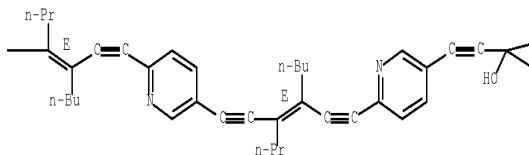
pyridinyl]ethynyl]-3-hepten-1-yn-1-yl]-3-pyridinyl]-2-methyl- (CA INDEX NAME)

Double bond geometry as shown.

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PAGE 1-C

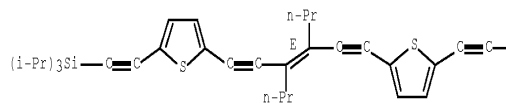


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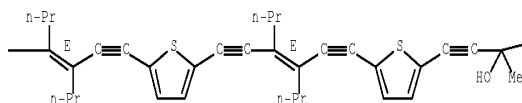
CN 3-Butyn-2-ol, 4-[5-[(3E)-4-[2-[5-[(3E)-5-ethyl-4-[2-[5-[(3E)-5-ethyl-3-propyl-4-[2-[5-[2-[tris(1-methylethyl)silyl]ethynyl]-2-thienyl]ethynyl]-3-penten-1-yn-1-yl]-2-thienyl]ethynyl]-3-propyl-3-penten-1-yn-1-yl]-2-thienyl]ethynyl]-3-propyl-3-hepten-1-yn-1-yl]-2-thienyl]-2-methyl- (CA INDEX NAME)

Double bond geometry as shown.

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PAGE 1-B



PAGE 1-C

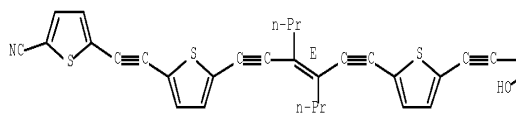


RN 864684-03-7 CAPLUS

CN 2-Thiophenecarbonitrile, 5-[2-[5-[(3E)-5-ethyl-4-[2-[5-(3-hydroxy-3-methyl-1-butyn-1-yl)-2-thienyl]ethynyl]-3-propyl-3-penten-1-yn-1-yl]-2-thienyl]ethynyl]- (CA INDEX NAME)

Double bond geometry as shown.

PAGE 1-A



PAGE 1-B

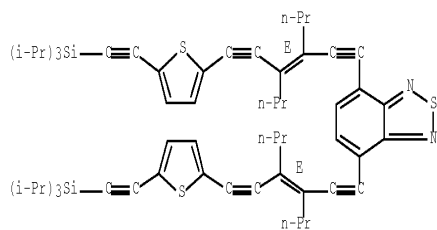


RN 864684-06-0 CAPLUS

CN 2,1,3-Benzothiadiazole, 4-[(3E)-3,4-dipropyl-6-[5-[2-[tris(1-methylethyl)silyl]ethynyl]-2-thienyl]-3-hexene-1,5-diyn-1-yl]-7-[(3E)-3-propyl-4-[2-[5-[2-[tris(1-methylethyl)silyl]ethynyl]-2-thienyl]ethynyl]-3-hepten-1-yn-1-yl]- (CA INDEX NAME)

Double bond geometry as shown.





RN 864684-22-0 CAPLUS

CN Benzene, 1-[(3E)-3,4-dipropyl-6-[4-[2-[tris(1-methylethyl)silyl]ethynyl]phenyl]-3-hexene-1,5-diyn-1-yl]-4-[(3E)-3-propyl-4-[2-[4-[2-[tris(1-methylethyl)silyl]ethynyl]phenyl]ethynyl]-3-hepten-1-yn-1-yl]- (CA INDEX NAME)

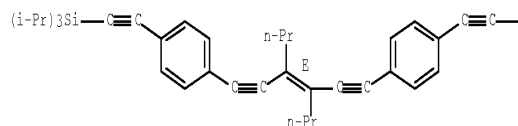
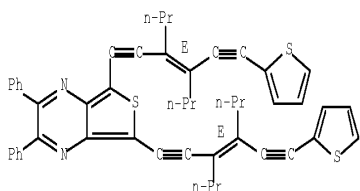
Double bond geometry as shown.

PAGE 1-A

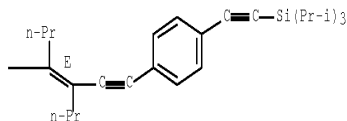
RN 864684-09-3 CAPLUS

CN Thieno[3,4-b]pyrazine, 5-[(3E)-3,4-dipropyl-6-(2-thienyl)-3-hexene-1,5-diyn-1-yl]-2,3-diphenyl-7-[(3E)-3-propyl-4-[2-(2-thienyl)ethynyl]-3-hepten-1-yn-1-yl]- (CA INDEX NAME)

Double bond geometry as shown.



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RN 864684-21-9 CAPLUS

CN Thiophene, 2-[(3E)-3,4-dipropyl-6-[4-[(3E)-3-propyl-4-[2-[5-[2-[tris(1-methylethyl)silyl]ethynyl]-2-thienyl]ethynyl]-3-hepten-1-yn-1-yl]phenyl]-3-hexene-1,5-diyn-1-yl]-5-[2-[tris(1-methylethyl)silyl]ethynyl]- (CA INDEX NAME)

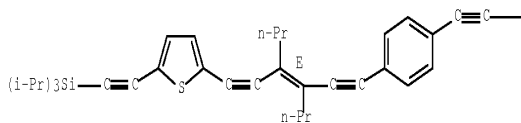
Double bond geometry as shown.

RN 864684-23-1 CAPLUS

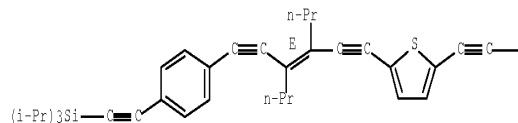
CN Thiophene, 2-[(3E)-3,4-dipropyl-6-[4-[2-[tris(1-methylethyl)silyl]ethynyl]phenyl]-3-hexene-1,5-diyn-1-yl]-5-[(3E)-3-propyl-4-[2-[4-[2-[tris(1-methylethyl)silyl]ethynyl]phenyl]ethynyl]-3-hepten-1-yn-1-yl]- (CA INDEX NAME)

Double bond geometry as shown.

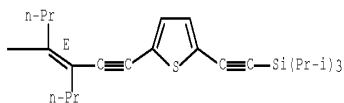
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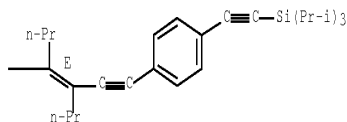
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PAGE 1-B



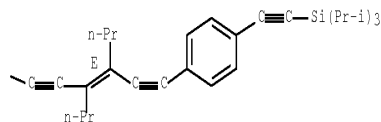




RN 864684-24-2 CAPLUS

CN Silane, [oxybis[4,1-phenylene[(3E)-3,4-dipropyl-3-hexene-1,5-diyne-6,1-diyl]-4,1-phenylene-2,1-ethynediyl]]bis[tris(1-methylethyl)- (9CI) (CA INDEX NAME)

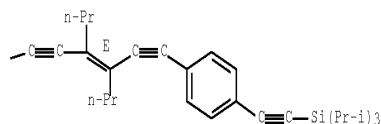
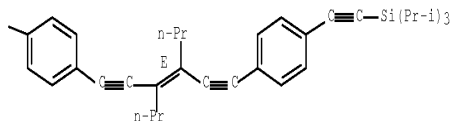
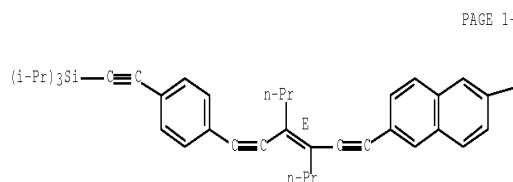
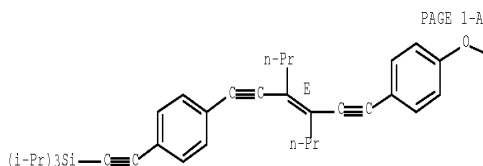
Double bond geometry as shown.



RN 864684-26-4 CAPLUS

CN Naphthalene, 2-[(3E)-3,4-dipropyl-6-[4-[2-[tris(1-methylethyl)silyl]ethynyl]phenyl]-3-hexene-1,5-diyn-1-yl]-6-[(3E)-3-propyl-4-[2-[4-[2-[tris(1-methylethyl)silyl]ethynyl]phenyl]ethynyl]-3-hepten-1-yn-1-yl]- (CA INDEX NAME)

Double bond geometry as shown.



RN 864684-25-3 CAPLUS

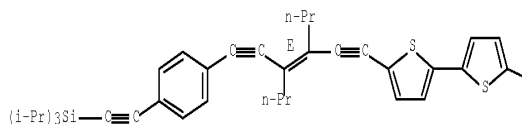
CN 2,2'-Bithiophene, 5-[(3E)-3,4-dipropyl-6-[4-[2-[tris(1-methylethyl)silyl]ethynyl]phenyl]-3-hexene-1,5-diyn-1-yl]-5'-[(3E)-3-propyl-4-[2-[4-[2-[tris(1-methylethyl)silyl]ethynyl]phenyl]ethynyl]-3-hepten-1-yn-1-yl]- (CA INDEX NAME)

Double bond geometry as shown.

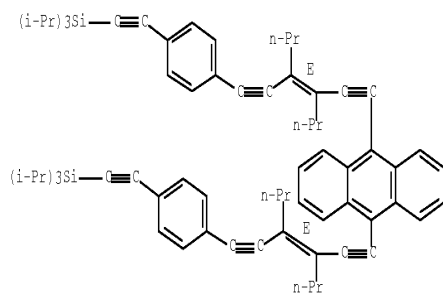
RN 864684-27-5 CAPLUS

CN Anthracene, 9-[(3E)-3,4-dipropyl-6-[4-[2-[tris(1-methylethyl)silyl]ethynyl]phenyl]-3-hexene-1,5-diyn-1-yl]-10-[(3E)-3-propyl-4-[2-[4-[2-[tris(1-methylethyl)silyl]ethynyl]phenyl]ethynyl]-3-hepten-1-yn-1-yl]- (CA INDEX NAME)

Double bond geometry as shown.



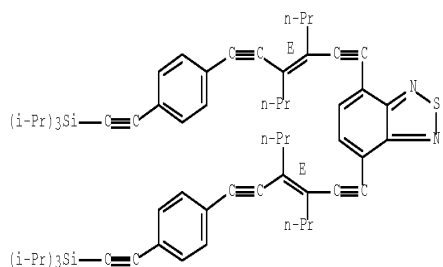




RN 864684-28-6 CAPLUS

CN 2,1,3-Benzothiadiazole, 4-[(3E)-3,4-dipropyl-6-[4-[2-[tris(1-methylethyl)silyl]ethynyl]phenyl]-3-hexene-1,5-diyn-1-yl]-7-[(3E)-3-propyl-4-[2-[4-[2-[tris(1-methylethyl)silyl]ethynyl]phenyl]ethynyl]-3-hepten-1-yn-1-yl]- (CA INDEX NAME)

Double bond geometry as shown.

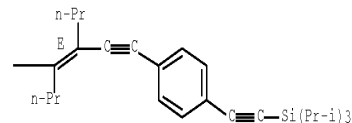
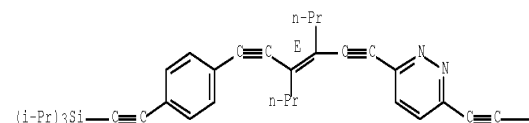


RN 864684-29-7 CAPLUS

CN Pyridazine, 3-[(3E)-3,4-dipropyl-6-[4-[2-[tris(1-methylethyl)silyl]ethynyl]phenyl]-3-hexene-1,5-diyn-1-yl]-6-[(3E)-3-propyl-4-[2-[4-[2-[tris(1-methylethyl)silyl]ethynyl]phenyl]ethynyl]-3-hepten-1-yn-1-yl]- (CA INDEX NAME)

Double bond geometry as shown.

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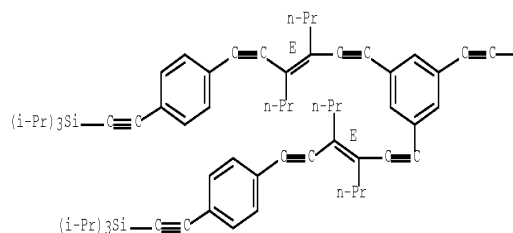


RN 864684-30-0 CAPLUS

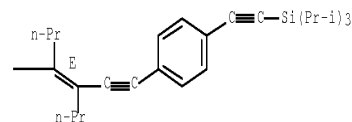
CN Benzene, 1-[(3E)-3,4-dipropyl-6-[4-[2-[tris(1-methylethyl)silyl]ethynyl]phenyl]-3-hexene-1,5-diyn-1-yl]-3-[(3E)-5-ethyl-3-propyl-4-[2-[4-[2-[tris(1-methylethyl)silyl]ethynyl]phenyl]ethynyl]-3-penten-1-yn-1-yl]-5-[(3E)-3-propyl-4-[2-[4-[2-[tris(1-methylethyl)silyl]ethynyl]phenyl]ethynyl]-3-hepten-1-yn-1-yl]- (CA INDEX NAME)

Double bond geometry as shown.

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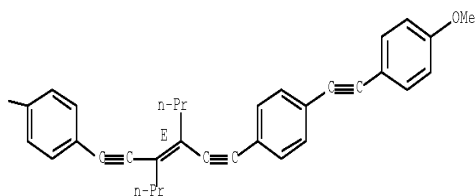
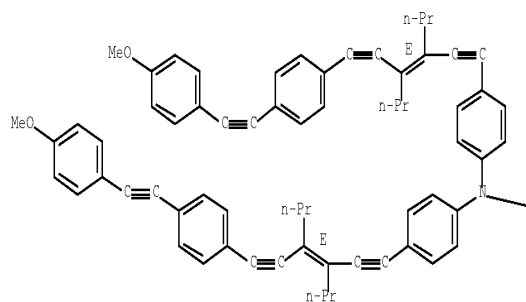


RN 864684-33-3 CAPLUS

CN Benzenamine, N-[4-[(3E)-5-ethyl-4-[2-[4-[2-(4-methoxyphenyl)ethynyl]phenyl]ethynyl]-3-propyl-3-penten-1-yn-1-yl]phenyl]-4-[(3E)-4-[2-[4-[2-(4-methoxyphenyl)ethynyl]phenyl]ethynyl]-3-propyl-3-hepten-1-yn-1-yl]-N-[4-[(3E)-4-[2-[4-[2-(4-methoxyphenyl)ethynyl]phenyl]ethynyl]-3-propyl-3-hepten-1-yn-1-yl]phenyl]- (CA INDEX NAME)

Double bond geometry as shown.





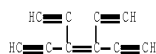
REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 3 OF 6 CAPLUS COPYRIGHT 2009 ACS on STN  
 ACCESSION NUMBER: 2003:739778 CAPLUS [Full-text](#)  
 DOCUMENT NUMBER: 139:388935  
 TITLE: Functional conjugated materials for optonics and electronics by tetraethynylethene molecular scaffolding  
 AUTHOR(S): Nielsen, Mogens Brondsted; Diederich, Francois  
 CORPORATE SOURCE: Laboratorium fuer Organische Chemie, HCI, ETH Honggerberg, Zurich, CH-8093, Switz.  
 SOURCE: Modern Arene Chemistry (2002), 196-216. Editor(s): Astruc, Didier. Wiley-VCH Verlag GmbH & Co. KGaA: Weinheim, Germany.  
 CODEN: 69EMIX; ISBN: 3-527-30489-4  
 DOCUMENT TYPE: Conference; General Review  
 LANGUAGE: English  
 AB A review; the phys. properties of scaffolds based on tetraethynylethene (TEE; 3,4-diethynylhex-3-ene-1,5-diyne) are strongly enhanced by arylation. Indeed, owing to the coplanarity of anilino-substituted TEE scaffolds, very high

third-order optical nonlinearities are obtained. Moreover, arylated TEEs are able to undergo photochem. induced cis-trans isomerization, paving the way for applications as light-driven mol. switches in optoelectronic devices. Suitably functionalized TEE modules are readily incorporated into linear and cyclic n-conjugated scaffolds, employing stepwise acetylenic coupling protocols. Thus, TEE mol. scaffolding has provided access to large, macrocyclic, all-carbon cores and long poly(triacetylene) (PTA) oligomers.

IT 133968-85-1D, Tetraethynylethene, aryl derivs.  
 RL: DEV (Device component use); USES (Uses)  
 (functional conjugated materials for optonics and electronics by tetraethynylethene mol. scaffolding)

RN 133968-85-1 CAPLUS  
 CN 3-Hexene-1,5-diyne, 3,4-diethynyl- (CA INDEX NAME)



OS.CITING REF COUNT: 14 THERE ARE 14 CAPLUS RECORDS THAT CITE THIS RECORD (14 CITINGS)  
 REFERENCE COUNT: 110 THERE ARE 110 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 4 OF 6 CAPLUS COPYRIGHT 2009 ACS on STN  
 ACCESSION NUMBER: 2003:189466 CAPLUS [Full-text](#)  
 DOCUMENT NUMBER: 139:101213  
 TITLE: Luminescent properties of carbon-rich starburst gold(I) acetylide complexes. Crystal structure of [TEE][Au(PCy3)]4 ([TEE]H4 = tetraethynylethene)  
 AUTHOR(S): Lu, Wei; Zhu, Nianying; Che, Chi-Ming  
 CORPORATE SOURCE: Department of Chemistry and HKU-CAS Joint Laboratory on New Materials, The University of Hong Kong, Hong Kong, Peop. Rep. China  
 SOURCE: Journal of Organometallic Chemistry (2003), 670(1-2), 11-16  
 CODEN: JORCAI; ISSN: 0022-328X  
 PUBLISHER: Elsevier Science B.V.  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 OTHER SOURCE(S): CASREACT 139:101213  
 AB Two carbon-rich starburst gold(I) acetylide complexes [TEE][Au(PCy3)]4 (3, [TEE]H4 = tetraethynylethene) and [TEB][Au(PCy3)]3 (6, [TEB]H3 = 1,3,5-triethynylbenzene) were prepared and their UV-vis absorption, emission and excitation spectra have been recorded. In fluid CH2Cl2 solns., 3 exhibits prompt 1(ππ\*) fluorescence with λ0-0 and λmax at 413 and 428 nm, resp., while 6 displays 3(ππ\*) phosphorescence with λ0-0 and λmax at 446 and 479 nm, resp. The crystal structure of 3·CH2Cl2 has been determined  
 IT 553469-17-8P  
 RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)  
 (crystal structure; preparation and luminescent properties of carbon-rich starburst gold acetylide complexes and crystal structure of tetraethynylethene gold phosphine complex)  
 RN 558460-17-6 CAPLUS  
 CN Gold, [μ-[3,4-di(ethynyl)-KC2]-3-hexene-1,5-diyne(4)-]



KCl,KC6]]tetrakis(tricyclohexylphosphine)tetra-, compd. with dichloromethane (1:1) (9CI) (CA INDEX NAME)

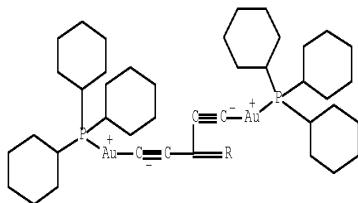
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CRN 558460-16-5

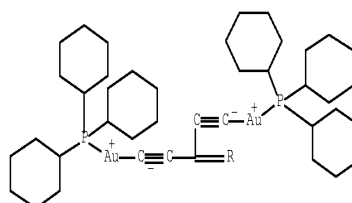
CMF C82 H132 Au4 P4

CCI CCS

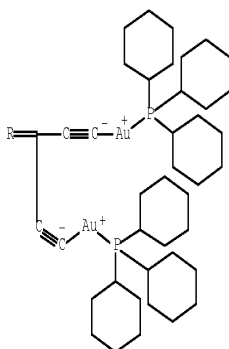
PAGE 1-A



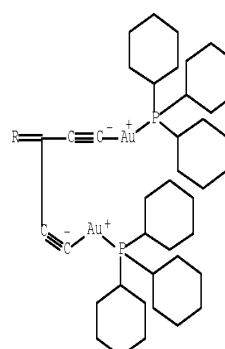
PAGE 1-A



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CM 2

CRN 75-09-2

CMF C H2 Cl2

C1=CH2=C1

IT 558460-16-5P

RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation) (mol. structure, luminescence; preparation and luminescent properties of carbon-rich starburst gold acetylide complexes and crystal structure of tetraethynylethene gold phosphine complex)

RN 558460-16-5 CAPLUS

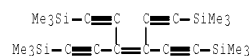
CN Gold, [μ-[3,4-di(ethynyl-κC2)-3-hexene-1,5-diynato(4-)-κC1,κC6]]tetrakis(tricyclohexylphosphine)tetra- (9CI) (CA INDEX NAME)

IT 55660-76-9

RL: RCT (Reactant); RACT (Reactant or reagent) (preparation and luminescent properties of carbon-rich starburst gold acetylide complexes and crystal structure of tetraethynylethene gold phosphine complex)

RN 55660-76-9 CAPLUS

CN Silane, 1,1'-[3,4-bis[2-(trimethylsilyl)ethynyl]-3-hexene-2,5-diyne-1,6-diyl]bis[1,1,1-trimethyl- (CA INDEX NAME)





OS.CITING REF COUNT: 30 THERE ARE 30 CAPLUS RECORDS THAT CITE THIS RECORD (30 CITINGS)

REFERENCE COUNT: 34 THERE ARE 34 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 5 OF 6 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 2001:240433 CAPLUS [Full-text](#)

DOCUMENT NUMBER: 135:19763

TITLE: Pt-tetraethynylethene molecular scaffolding: synthesis and characterization of a novel class of organometallic molecular rods

AUTHOR(S): Siemsen, Peter; Gubler, Ulrich; Bosshard, Christian; Gunter, Peter; Diederich, Francois

CORPORATE SOURCE: Laboratorium fur Organische Chemie, ETH-Zentrum, Zurich, 8092, Switz.

SOURCE: Chemistry--A European Journal (2001), 7(6), 1333-1341  
CODEN: CEUJED; ISSN: 0947-6539

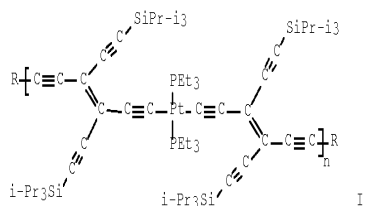
PUBLISHER: Wiley-VCH Verlag GmbH

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 135:19763

GI



AB The series of monodisperse Pt-bridged TEE oligomers I (R = C.tplbond.CPh; n = 1-6) was prepared by oxidative Glaser - Hay oligomerization of monomer 7 under endcapping conditions. These novel mol. rods extend in length from 3.3 nm to 12.1 nm. Their isolation was achieved by high performance gel permeation chromatog. (GPC), and their purification was best monitored by anal. GPC in combination with matrix-assisted laser-desorption-ionization mass spectrometry (MALDI-TOF MS). The mass spectra of each oligomer revealed the mol. ion or its sodium complex as parent ion together with a clean, highly characteristic fragmentation pattern. Delayed addition of the end-capping reagent PhCCH to the oligomerization mixture afforded polymer I (R = H; n = 1) with an average of  $\approx 32$  repeat units and a remarkably narrow mol. weight distribution ( $M_w/M_n = 1.06$ ), which is indicative of a living polymerization process. UV/Vis spectral data as well as measurements of the second hyperpolarizability  $\gamma$  by third harmonic generation (THG) revealed a nearly complete lack of  $\pi$ -electron delocalization along the oligomeric backbone. The Pt atoms act as true insulating centers, and the Pt-C(sp) bonds hardly possess any  $\pi$  character. The synthesis of the mol. rods I provides another demonstration of the power of oxidative acetylenic homocouplings for the preparation of unusual nanoarchitecture.

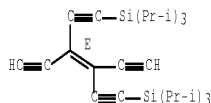
IT 155063-39-1

RL: RCT (Reactant); RACT (Reactant or reagent)  
(Hagihara coupling of)

RN 155063-39-1 CAPLUS

CN Silane, 1,1'-[(3E)-3,4-diethynyl-3-hexene-1,5-diyne-1,6-diyl]bis[1,1,1-tris(1-methylethyl)- (CA INDEX NAME)

Double bond geometry as shown.



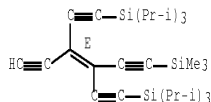
IT 177500-66-2

RL: RCT (Reactant); RACT (Reactant or reagent)  
(Hagihara coupling of, to form corresponding platinum bis(acetylide) complex)

RN 177500-66-2 CAPLUS

CN Silane, [(3E)-3-ethynyl-4-[(trimethylsilyl)ethynyl]-3-hexene-1,5-diyne-1,6-diyl]bis[tris(1-methylethyl)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

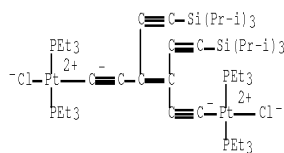


IT 342885-85-2P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(failed reaction; preparation and attempted oligomerization of)

RN 342885-85-2 CAPLUS

CN Platinum, [ $\mu$ -[(3E)-3,4-bis[[tris(1-methylethyl)silyl]ethynyl]-3-hexene-1,5-diyne-1,6-diyl]]dichlorotetrakis(triethylphosphine)di-, stereoisomer (9CI) (CA INDEX NAME)



IT 342885-86-5P

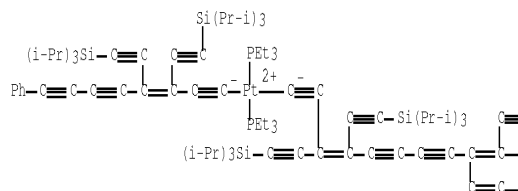
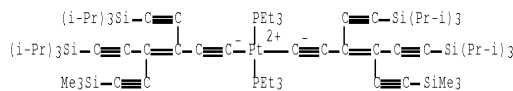
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(preparation and desilylation of)



RN 342885-88-5 CAPLUS

CN Platinum, bis(triethylphosphine)bis[(3Z)-6-(trimethylsilyl)-3,4-bis[[tris(1-methylethyl)silyl]ethynyl]-3-hexene-1,5-diynyl]-, (SP-4-1)-(9CI) (CA INDEX NAME)

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IT 342885-89-6[[P, terminated by phenylacetylene

342885-89-9P 342885-91-0P 342885-92-1P

RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)  
(preparation and nonlinear optical properties of)

RN 342885-89-6 CAPLUS

CN Platinum, bis[(3Z)-4-ethynyl-6-[tris(1-methylethyl)silyl]-3-[[tris(1-methylethyl)silyl]ethynyl]-3-hexene-1,5-diynyl]bis(triethylphosphine)-, (SP-4-1)-, homopolymer (9CI) (CA INDEX NAME)

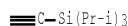
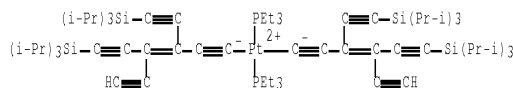
CM 1

PAGE 1-B

CRN 342885-86-3

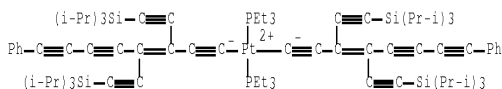
CMF C68 H116 P2 Pt Si4

CCI CCS



RN 342885-90-9 CAPLUS

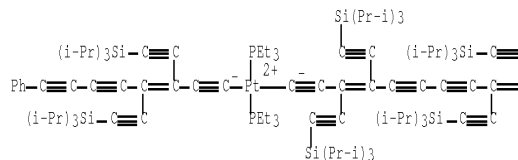
CN Platinum, bis[(3Z)-8-phenyl-3,4-bis[[tris(1-methylethyl)silyl]ethynyl]-3-octene-1,5,7-triynyl]bis(triethylphosphine)-, (SP-4-1)-(9CI) (CA INDEX NAME)



RN 342885-92-1 CAPLUS

CN Platinum, bis[(3Z)-8-phenyl-3,4-bis[[tris(1-methylethyl)silyl]ethynyl]-3-octene-1,5,7-triynyl]bis[μ-[(3Z,9Z)-3,4,9,10-tetrakis[[tris(1-methylethyl)silyl]ethynyl]-3,9-dodecadiene-1,5,7,11-tetrayne-1,12-diyl]]hexakis(triethylphosphine)tri-, stereoisomer (9CI) (CA INDEX NAME)

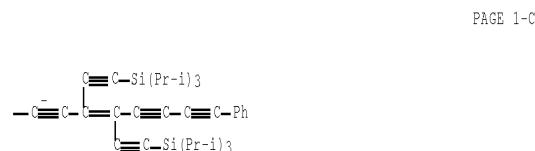
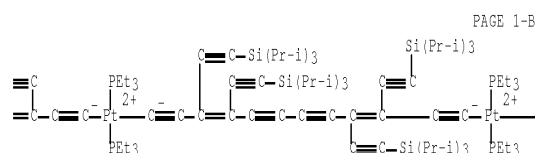
PAGE 1-A



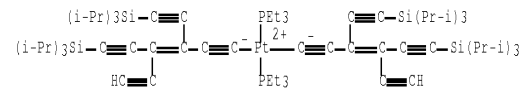
RN 342885-91-0 CAPLUS

CN Platinum, bis[(3Z)-8-phenyl-3,4-bis[[tris(1-methylethyl)silyl]ethynyl]-3-octene-1,5,7-triynyl][μ-[(3Z,9Z)-3,4,9,10-tetrakis[[tris(1-methylethyl)silyl]ethynyl]-3,9-dodecadiene-1,5,7,11-tetrayne-1,12-diyl]]tetrakis(triethylphosphine)di-, stereoisomer (9CI) (CA INDEX NAME)





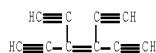
IT 342885-86-3P  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
 (preparation and oxidative Glaser-Hay oligomerization of)  
 RN 342885-86-3 CAPLUS  
 CN Platinum, bis[(3Z)-4-ethynyl-6-[tris(1-methylethyl)silyl]-3-[[tris(1-methylethyl)silyl]ethynyl]-3-hexene-1,5-diynyl]bis(triethylphosphine)-, (SP-4-1)- (9CI) (CA INDEX NAME)



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 REFERENCE COUNT: 76 THERE ARE 76 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 6 OF 6 CAPLUS COPYRIGHT 2009 ACS ON STN  
 ACCESSION NUMBER: 1999:370934 CAPLUS [Full-text](#)  
 DOCUMENT NUMBER: 131:31961  
 TITLE: Tetraethynylethenes: versatile carbon-rich building blocks for two-dimensional acetylenic scaffolding  
 AUTHOR(S): Diederich, Francois  
 CORPORATE SOURCE: Department of Chemistry, Swiss Federal Institute of Technology, Zurich, CH-8092, Switz.  
 SOURCE: NATO ASI Series, Series C: Mathematical and Physical Sciences (1997), 499(Modular Chemistry), 17-31  
 CODEN: NSCSDW; ISSN: 0258-2023  
 PUBLISHER: Kluwer Academic Publishers  
 DOCUMENT TYPE: Journal; General Review

LANGUAGE: English  
 AB Derivs. of tetraethynylethene (TEE, 3,4-diethynyl-hex-3-ene-1,5-diyne) constitute a versatile mol. construction kit for acetylenic mol. scaffolding. TEEs were introduced into multinanometer-sized functional mol. and polymeric materials with stable, extended C cores that exhibit unusual electronic and optical properties. The planar TEE C frame is a basic repeat unit for the construction of two-dimensional crystalline all-C networks. Starting from cisbis-deprotected TEEs, annulenes were prepared as macrocyclic precursors to such networks. The challenges encountered in the formation of extended regular C networks by oxidative acetylenic coupling are discussed, and techniques from supramol. chemical probably overcome the difficulties that prevented their preparation so far. One approach consists in the self-assembly of metal-acetylenic networks under thermodyn. control and error checking, followed by reductive elimination of the metal centers to the all-C net. Expanded radialenes represent another class of stable, extended C-rich compds. which were prepared for the 1st time starting from TEE precursors. Trans-bis-deprotected TEEs provided access to rod-like oligomers and polymers with the novel polytriacyetylene (PTA) backbone. The redox-properties of these remarkably stable materials are discussed. Tetrakis(phenylethynyl)ethene forms highly ordered charge-transfer complexes with  $\Pi$ -acceptors in the solid state and in solution. By attaching p-donor and p-acceptor substituted Ph rings to TEEs, novel NLO materials were obtained. It was shown for a large class of TEEs that donor/acceptor substitutions and fully two-dimensional conjugation strongly enhance the 3rd-order nonlinear optical properties. The relevance of the results obtained from studies of extended unsatd. C-rich materials for C allotropy in general is discussed. A review with 30 refs.  
 IT 133968-85-10P, Tetraethynylethene, organic derivs.  
 RL: PEP (Physical, engineering or chemical process); PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); PROC (Process); RACT (Reactant or reagent)  
 (as versatile carbon-rich building blocks for two-dimensional acetylenic scaffolding)  
 RN 133968-85-1 CAPLUS  
 CN 3-Hexene-1,5-diyne, 3,4-diethynyl- (CA INDEX NAME)



OS.CITING REF COUNT: 1 THERE ARE 1 CAPLUS RECORDS THAT CITE THIS RECORD (1 CITINGS)  
 REFERENCE COUNT: 55 THERE ARE 55 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

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